ACCESS DB # 21134?2

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Scientific and Technical Information Center

SEARCH REQUEST FORM

Requester's Full Name: MARK BERCH Examiner # : 59193 Date: 3/6/07

Art Unit: 1624 Phone Number: 2- 0663 Serial Number: 10500451

Location (Bldg/Room#): 5C01 (Mailbox #): 5C18 Results Format Preferred (circle): PAPER DISK

****

To ensure an efficient and quality search, please attach a copy of the cover sheet, claims, and abstract or fill out the following:

Title of Invention: _____

Inventors (please provide full names): _____

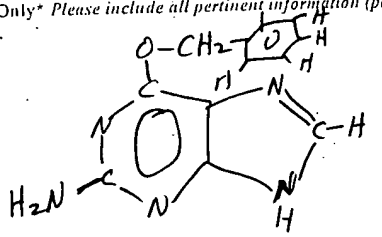
03-296

Earliest Priority Date: _____

Search Topic:

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc., if known.

For Sequence Searches Only *Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.*



Note: No fuq sts

2 Searches

(A) Any ref with this cmpd as multicomponent

(B) Synthesis of this cmpd.

****

STAFF USE ONLY

Searcher: _____

Searcher Phone #: _____

Searcher Location: _____

Date Searcher Picked Up: _____

Date Completed: _____

Searcher Prep & Review Time: _____

Online Time: _____

Type of Search

_____ NA Sequence (#)

_____ AA Sequence (#)

_____ Structure (#)

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_____ Litigation

_____ Fulltext

_____ Other

Vendors and cost where applicable

_____ STN _____ Dialog

_____ Questel/Orbit _____ Lexis/Nexis

_____ Westlaw _____ WWW/Internet

____ In-house sequence systems

__ Commercial ___ Oligomer ____ Score/Length

__ Interference ___ SPDI ____ Encode/Transl

_____ Other (specify)

=> file registry
FILE 'REGISTRY' ENTERED AT 11:10:41 ON 09 MAR 2007
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STRUCTURE FILE UPDATES: 8 MAR 2007 HIGHEST RN 925886-00-6
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FILE COVERS 1907 - 9 Mar 2007 VOL 146 ISS 12
FILE LAST UPDATED: 8 Mar 2007 (20070308/ED)

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They are available for your review at:

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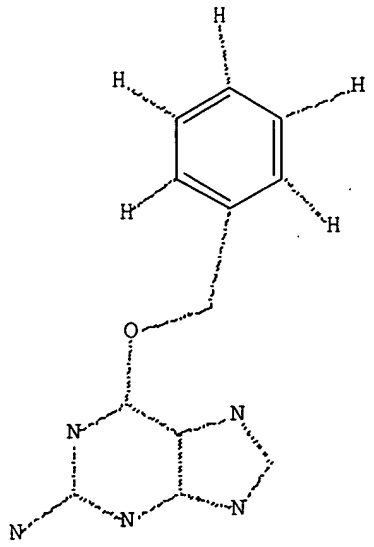
=> d stat que L6
L1 STR



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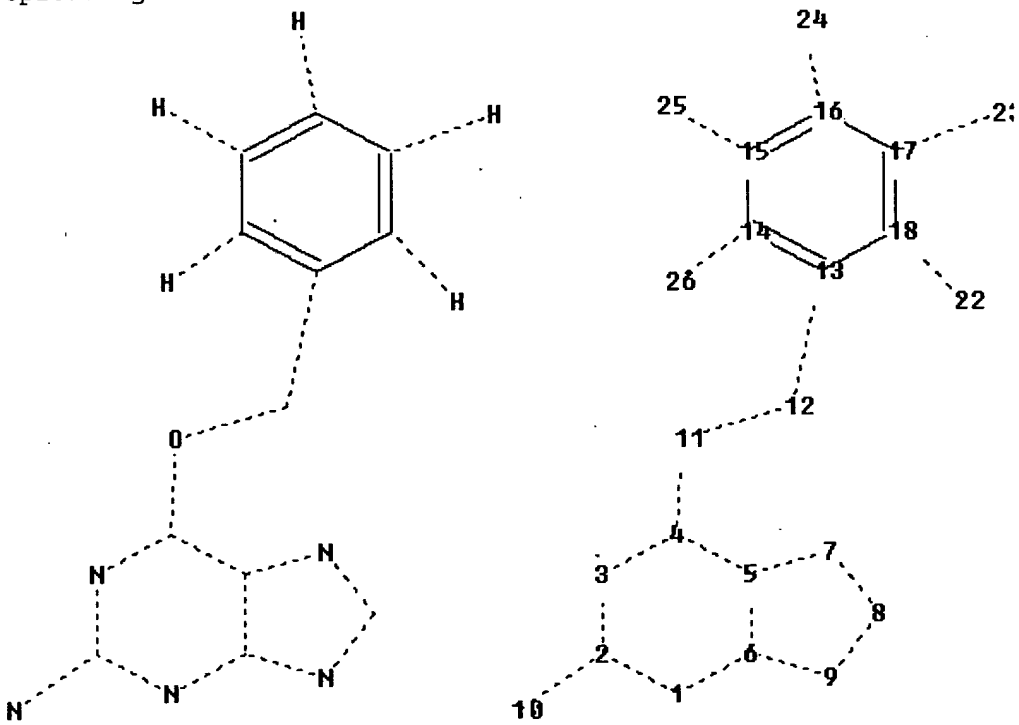

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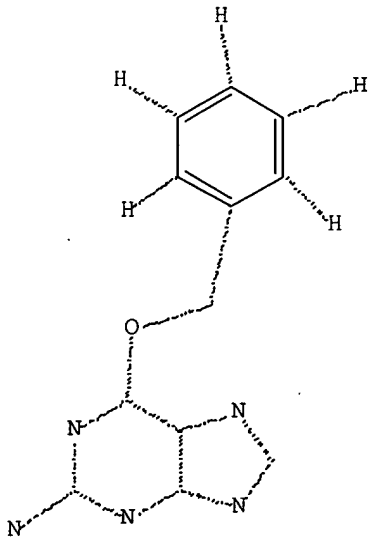
10 11 12 22 23 24 25 26
ring nodes :
1 2 3 4 5 6 7 8 9 13 14 15 16 17 18
chain bonds :
2-10 4-11 11-12 12-13 14-26 15-25 16-24 17-23 18-22
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 13-14 13-18 14-15 15-16 16-17

17-18
exact/norm bonds :
1-2 1-6 2-3 2-10 3-4 4-5 4-11 5-6 5-7 6-9 7-8 8-9 11-12 12-13 14-26
15-25 16-24 17-23 18-22
normalized bonds :
13-14 13-18 14-15 15-16 16-17 17-18

Connectivity :
1:2 E exact RC ring/chain 2:3 E exact RC ring/chain 3:2 E exact RC ring/chain
4:3 E exact RC ring/chain 5:3 E exact RC ring/chain 6:3 E exact RC ring/chain
7:2 E exact RC ring/chain
8:2 E exact RC ring/chain 9:2 E exact RC ring/chain 10:1 E exact RC ring/chain
11:2 E exact
RC ring/chain 12:2 E exact RC ring/chain 13:3 E exact RC ring/chain
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:CLASS 12:CLASS 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 22:CLASS
23:CLASS 24:CLASS
25:CLASS 26:CLASS

L3 16 SEA FILE=REGISTRY SSS FUL L1
L4 1 SEA FILE=REGISTRY ABB=ON PLU=ON "9H-PURIN-2-AMINE, 6-(PHENYLM
ETHOXY)-"/CN
L5 15 SEA FILE=REGISTRY ABB=ON PLU=ON L3 NOT L4
L6 9 SEA FILE=CAPLUS ABB=ON PLU=ON L5

=> d stat que L11
L1 STR



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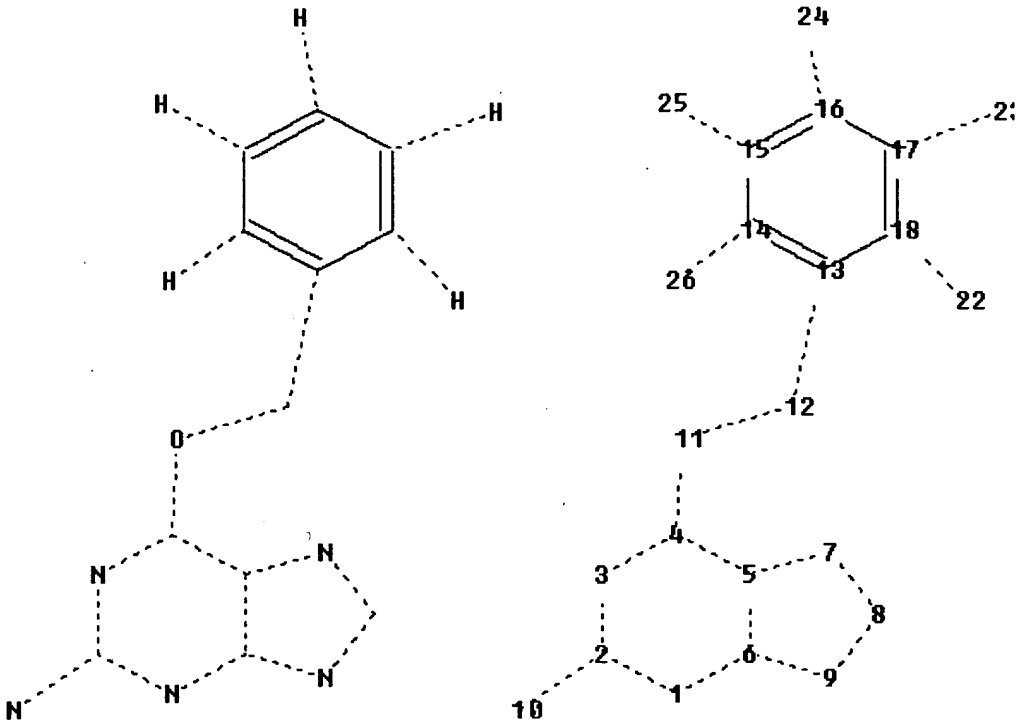

chain nodes :
10 11 12 22 23 24 25 26
ring nodes :
1 2 3 4 5 6 7 8 9 13 14 15 16 17 18
chain bonds :
2-10 4-11 11-12 12-13 14-26 15-25 16-24 17-23 18-22
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 13-14 13-18 14-15 15-16 16-17
17-18
exact/norm bonds :
1-2 1-6 2-3 2-10 3-4 4-5 4-11 5-6 5-7 6-9 7-8 8-9 11-12 12-13 14-26
15-25 16-24 17-23 18-22
normalized bonds :
13-14 13-18 14-15 15-16 16-17 17-18

Connectivity :
1:2 E exact RC ring/chain 2:3 E exact RC ring/chain 3:2 E exact RC ring/chain
4:3 E exact RC ring/chain 5:3 E exact RC ring/chain 6:3 E exact RC ring/chain
7:2 E exact RC ring/chain
8:2 E exact RC ring/chain 9:2 E exact RC ring/chain 10:1 E exact RC ring/chain
11:2 E exact
RC ring/chain 12:2 E exact RC ring/chain 13:3 E exact RC ring/chain
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:CLASS 12:CLASS 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 22:CLASS
23:CLASS 24:CLASS
25:CLASS 26:CLASS

L3 16 SEA FILE=REGISTRY SSS FUL L1
L4 1 SEA FILE=REGISTRY ABB=ON PLU=ON "9H-PURIN-2-AMINE, 6-(PHENYLM

```
                ETHOXY)-"/CN
L5             15 SEA FILE=REGISTRY ABB=ON  PLU=ON  L3 NOT L4
L6              9 SEA FILE=CAPLUS ABB=ON  PLU=ON  L5
L10            47 SEA FILE=CAPLUS ABB=ON  PLU=ON  L3/P
L11             6 SEA FILE=CAPLUS ABB=ON  PLU=ON  L10 AND L6


=> s L11 or L6
L14             9 L11 OR L6

=> => => d L14 ibib abs hitind hitstr L14 1-9
L14 IS NOT VALID HERE
For an explanation, enter "HELP DISPLAY".

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FILE 'CAPLUS' ENTERED AT 11:17:37 ON 09 MAR 2007
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FILE COVERS 1907 - 9 Mar 2007  VOL 146 ISS 12
FILE LAST UPDATED: 8 Mar 2007  (20070308/ED)

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=> d L14 ibib abs hitind hitstr 1-9

L14  ANSWER 1 OF 9  CAPLUS  COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER:         2006:39406  CAPLUS  Full-text
DOCUMENT NUMBER:          144:219195
TITLE:                    Combined antitumor medicines containing guanine
                          analogs and nitrosourea drugs for the treatment of
                          solid tumors
INVENTOR(S):              Kong, Qingzhong
PATENT ASSIGNEE(S):       Peop. Rep. China
SOURCE:                   Faming Zhuanli Shenqing Gongkai Shuomingshu, 21 pp.
                          CODEN: CNXXEV
DOCUMENT TYPE:            Patent
LANGUAGE:                 Chinese
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.           KIND   DATE        APPLICATION NO.         DATE
     ---------------      ----   --------    --------------------    --------
     CN 1628852            A     20050622    CN 2004-10035928        20041014
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PRIORITY APPLN. INFO.: CN 2004-10035928 20041014

AB The title medicines contain 0.01-70% guanine analogs or its derivs., 0-50% nitrosourea compds., and pharmaceutical auxiliary materials. The medicines can inhibit DNA repair in tumor cells, and reduce the drug resistance of tumor cells to nitrosourea anticancer drugs. The pharmaceutical auxiliary materials are biocompatible and biodegradable polymer, which can slowly release the anticancer active ingredients at the tumor site during the biodegrdn. and absorption process so as to reduce the systemic toxic reaction while maintaining effective levels of the drugs at the tumor site. The medicines can be placed at the tumor site to improve the therapeutic effect of non-operative therapy such as chemotherapy and radiotherapy.

IC ICM A61K045-06
ICS A61P035-00; A61K031-522

CC 63-6 (Pharmaceuticals)
Section cross-reference(s): 1

IT 66-75-1, Uramustine 73-40-5 73-40-5D, Guanine, 6-O-alkenyl derivs. 73-40-5D, Guanine, analogs 154-93-8, Carmustine 576-68-1, Mannomustine 578-76-7 2998-57-4, Estramustine 4552-61-8 6301-83-3 9033-25-4, Methyltransferase 13010-47-4, Lomustine 13909-09-6, Semustine 16506-27-7, Bendamustine 18883-66-4, Streptozotocin 19916-73-5, O6-Benzyl guanine 19916-74-6 20535-83-5 24937-78-8, Ethylene-vinyl acetate copolymer 26023-30-3, Poly[oxy(1-methyl-2-oxo-1,2-ethanediyl)] 29069-24-7, Prednimustine 34346-01-5, Glycolic acid-lactic acid copolymer 42471-28-3, Nimustine 55102-44-8, Bofumustine 56605-16-4, Spiromustine 57346-44-8 58994-96-0, Ranimustine 60784-46-5, Elmustine 64236-05-1 73105-03-0, Pentamustine 75219-46-4, Atrimustine 76412-62-9 81965-43-7 82599-22-2, Ditiomustine 85754-59-2, Ambamustine 85977-49-7, Tauromustine 92118-27-9, Fotemustine 98383-18-7, Ecomustine 105618-02-8, Galamustine 115308-98-0, Tallimustine 139402-18-9, Alestramustine 144084-41-3 158754-46-2 158754-46-2D, acetyl derivs. 158754-46-2D, diacetyl derivative 160948-23-2 160948-25-4 160948-27-6 160948-28-7 160948-29-8 160948-30-1 160948-31-2 160948-32-3 160948-34-5, 2,8-Diamino-6-chloropurine 177328-90-4 177328-92-6 177328-93-7 177328-94-8 177328-95-9 177328-96-0 188680-43-5, O6-(1-Cyclopentenylmethyl) guanine 192441-08-0 244246-55-7 307494-50-4 ***876054-46-5 876054-47-6 876054-48-7 876054-49-8 876054-50-1 876054-51-2 876054-52-3*** 876054-53-4
RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(combined antitumor compns. containing guanine analogs and nitrosourea drugs for the treatment of solid tumors)

IT ***876054-46-5 876054-47-6 876054-48-7 876054-49-8 876054-50-1 876054-51-2 876054-52-3***
RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(combined antitumor compns. containing guanine analogs and nitrosourea drugs for the treatment of solid tumors)

RN 876054-46-5 CAPLUS

CN Urea, N,N'-bis(2-chloroethyl)-N-nitroso-, mixt. with 6-(phenylmethoxy)-1H-purin-2-amine (9CI) (CA INDEX NAME)

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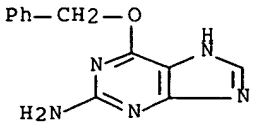

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CRN 154-93-8
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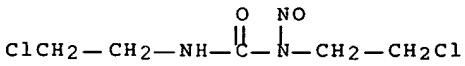

RN 876054-47-6 CAPLUS
CN Urea, N'-[(4-amino-2-methyl-5-pyrimidinyl)methyl]-N-(2-chloroethyl)-N-nitroso-, mixt. with 6-(phenylmethoxy)-1H-purin-2-amine (9CI) (CA INDEX NAME)

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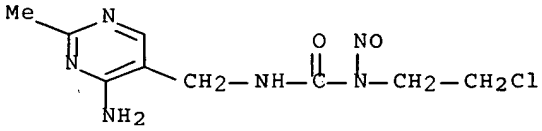
CRN 42471-28-3
CMF C9 H13 Cl N6 O2



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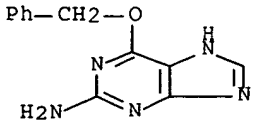

RN 876054-48-7 CAPLUS
CN Urea, N-(2-chloroethyl)-N'-cyclohexyl-N-nitroso-, mixt. with 6-(phenylmethoxy)-1H-purin-2-amine (9CI) (CA INDEX NAME)

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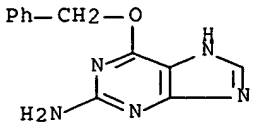
CRN 19916-73-5
CMF C12 H11 N5 O



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CRN 13010-47-4
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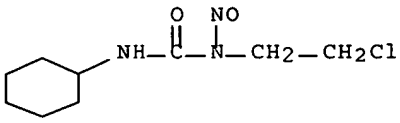

RN 876054-49-8 CAPLUS
CN Acetamide, 2-[[[(2-chloroethyl)nitrosoamino]carbonyl]methylamino]-, mixt. with 6-(phenylmethoxy)-1H-purin-2-amine (9CI) (CA INDEX NAME)

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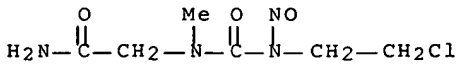
CRN 81965-43-7
CMF C6 H11 Cl N4 O3



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CRN 19916-73-5
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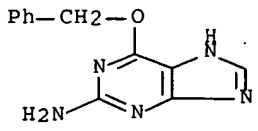

RN 876054-50-1 CAPLUS
CN Urea, N-(2-chloroethyl)-N'-cyclohexyl-N'-methyl-N-nitroso-, mixt. with 6-(phenylmethoxy)-1H-purin-2-amine (9CI) (CA INDEX NAME)

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CRN 64236-05-1
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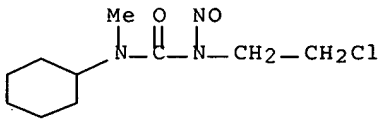

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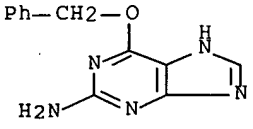
CMF C12 H11 N5 O



RN 876054-51-2 CAPLUS
CN D-Glucose, 2-deoxy-2-[[(methylnitrosoamino)carbonyl]amino]-, mixt. with 6-(phenylmethoxy)-1H-purin-2-amine (9CI) (CA INDEX NAME)

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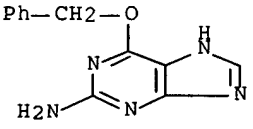
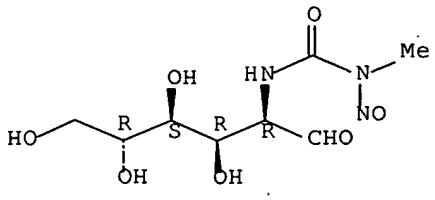


CM 2

CRN 18883-66-4
CMF C8 H15 N3 O7

Absolute stereochemistry.



RN 876054-52-3 CAPLUS
CN Urea, N-(2-chloroethyl)-N'-(4-methylcyclohexyl)-N-nitroso-, mixt. with 6-(phenylmethoxy)-1H-purin-2-amine (9CI) (CA INDEX NAME)

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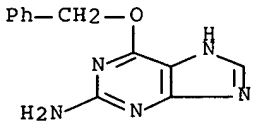
CRN 19916-73-5
CMF C12 H11 N5 O



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CRN 13909-09-6
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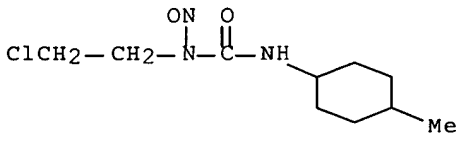


L14 ANSWER 2 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:818423 CAPLUS Full-text
DOCUMENT NUMBER: 139:307791
TITLE: Crystal polymorphism and crystal solvates of 2-amino-6-(benzyloxy)purine and process for their production
INVENTOR(S): Hayashi, Taketo; Kawakami, Takehiko; Iwanaga, Yoshihiko; Watanabe, Yosuke
PATENT ASSIGNEE(S): Sumika Fine Chemicals Co., Ltd., Japan
SOURCE: PCT Int. Appl., 36 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent

LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003084957	A1	20031016	WO 2003-JP4258	20030403
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2003226447	A1	20031020	AU 2003-226447	20030403
EP 1492791	A1	20050105	EP 2003-745892	20030403
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
US 2005080098	A1	20050414	US 2003-500451	20030403
JP 2005522482	T	20050728	JP 2003-582154	20030403
PRIORITY APPLN. INFO.:			JP 2002-105805 A	20020408
			WO 2003-JP4258 W	20030403

AB A crystallization method was described so as to provide a solvate [e.g., 2-amino-6-(benzyloxy)purine ethanolate], a cubic crystal, and a columnar crystal of 2-amino-6-(benzyloxy)purine (prepared by the etherification of 2-amino-6-chloropurine with benzyl alc.) by crystallization from a solvent containing at least one kind of solvent selected from: (1) alc. and water; (2) alc. (e.g., ethanol); or (3) a water-containing solvent. X-ray diffraction pattern data and DSC data is presented.

IC ICM C07D473-18

CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 75

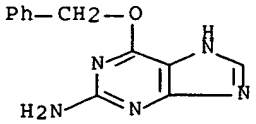
IT ***19916-73-5P***, 2-Amino-6-(benzyloxy)purine
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(crystal polymorphism and crystal solvates of 2-amino-6-(benzyloxy)purine and process for their production)

IT ***612507-54-7P 612507-56-9P 612507-59-2P***
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(crystal polymorphism and crystal solvates of 2-amino-6-(benzyloxy)purine and process for their production)

IT ***19916-73-5P***, 2-Amino-6-(benzyloxy)purine
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(crystal polymorphism and crystal solvates of 2-amino-6-(benzyloxy)purine and process for their production)

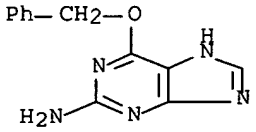
RN 19916-73-5 CAPLUS

CN 9H-Purin-2-amine, 6-(phenylmethoxy)- (CA INDEX NAME)



IT *612507-54-7P 612507-56-9P 612507-59-2P*
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(crystal polymorphism and crystal solvates of 2-amino-6-(benzyloxy)purine and process for their production)

RN 612507-54-7 CAPLUS
CN 1H-Purin-2-amine, 6-(phenylmethoxy)-, monohydrate (9CI) (CA INDEX NAME)

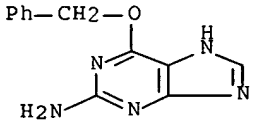


● H_2O

RN 612507-56-9 CAPLUS
CN Methanol, compd. with 6-(phenylmethoxy)-1H-purin-2-amine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 19916-73-5
CMF C12 H11 N5 O



CM 2

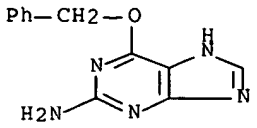
CRN 67-56-1
CMF C H4 O

$H_3C—OH$

RN 612507-59-2 CAPLUS
CN Ethanol, compd. with 6-(phenylmethoxy)-1H-purin-2-amine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 19916-73-5
CMF C12 H11 N5 O



CM 2

CRN 64-17-5
CMF C2 H6 O

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2000:213881 CAPLUS Full-text
DOCUMENT NUMBER: 133:17733
TITLE: New purine derivatives for efficient preparation of nucleoside analogs via alkylation
AUTHOR(S): Lukin, Kirill A.; Yang, ChengXi; Bellettini, John R.; Narayanan, B. A.
CORPORATE SOURCE: Process Development, Chemical and Agricultural Products Division, Abbott Laboratories, North Chicago, IL, 60064-6291, USA
SOURCE: Nucleosides, Nucleotides & Nucleic Acids (2000), 19(4), 815-825
CODEN: NNNAFY; ISSN: 1525-7770
PUBLISHER: Marcel Dekker, Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 133:17733

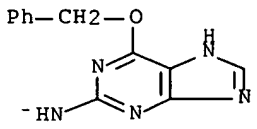
AB New diazabicycloundecenium and phosphazenium derivs. of purines are introduced for mild and efficient preparation of nucleoside analogs via in situ alkylation. Diazabicycloundecenium salts of purines were obtained directly as a result of an unusual reaction between two corresponding amino compds.

CC 33-9 (Carbohydrates)
IT 452-06-2, 2-Aminopurine 3558-06-3 6674-22-2, DBU 10310-21-1 19916-73-5 156126-50-0 ***163928-90-3*** 195157-22-3 273202-53-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(purine derivs. for efficient preparation of nucleoside analogs via alkylation)
IT 256949-27-6P ***256949-28-7P*** 256949-29-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(purine derivs. for efficient preparation of nucleoside analogs via alkylation)
IT ***163928-90-3***
RL: RCT (Reactant); RACT (Reactant or reagent)
(purine derivs. for efficient preparation of nucleoside analogs via

alkylation)
RN 163928-90-3 CAPLUS
CN 1-Butanaminium, N,N,N-tributyl-, salt with 6-(phenylmethoxy)-1H-purin-2-amine (1:1) (9CI) (CA INDEX NAME)

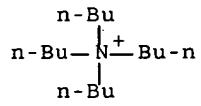
CM 1

CRN 163928-89-0
CMF C12 H10 N5 O



CM 2

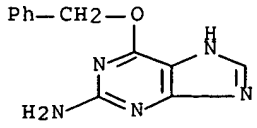
CRN 10549-76-5
CMF C16 H36 N



IT *256949-28-7P*
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(purine derivs. for efficient preparation of nucleoside analogs via alkylation)
RN 256949-28-7 CAPLUS
CN 1H-Purin-2-amine, 6-(phenylmethoxy)-, compd. with 2,3,4,6,7,8,9,10-octahydropyrimido[1,2-a]azepine (1:1) (9CI) (CA INDEX NAME)

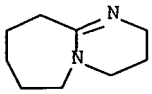
CM 1

CRN 19916-73-5
CMF C12 H11 N5 O



CM 2

CRN 6674-22-2
CMF C9 H16 N2



REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

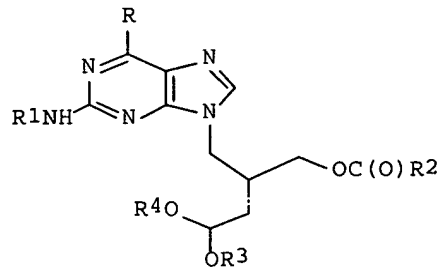
L14 ANSWER 4 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2000:117053 CAPLUS Full-text
DOCUMENT NUMBER: 132:137669
TITLE: Synthesis of acyclic nucleoside derivatives via alkylation reaction
INVENTOR(S): Leanna, M. Robert; Hannick, Steven M.; Rasmussen, Michael; Tien, Jien-heh J.; Bhagavatula, Lakshmi; Singam, Pulla Reddy; Gates, Bradley D.; Kolaczkowski, Lawrence; Patel, Ramesh R.; Wayne, Greg; Lannoyè, Greg; Zhang, Weijiang; Lukin, Kirill A.; Narayanan, Bikshandarkor; Riley, David A.; Morton, Howard; Chang, Sou-jen; Curty, Cynthia B.; Plata, Daniel; Bellettini, John; Shellat, Bhadra; Spitz, Tiffany; Yang, Cheng-xi
PATENT ASSIGNEE(S): Medivir AB, Swed.
SOURCE: PCT Int. Appl., 92 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 5
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000008025	A1	20000217	WO 1999-SE1339	19990805
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 6184376	B1	20010206	US 1998-130214	19980806
CA 2339250	A1	20000217	CA 1999-2339250	19990805
AU 9961271	A	20000228	AU 1999-61271	19990805
AU 765286	B2	20030911		
EP 1131323	A1	20010912	EP 1999-948005	19990805
EP 1131323	B1	20050427		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
JP 2002522439	T	20020723	JP 2000-563658	19990805
AT 294179	T	20050515	AT 1999-948005	19990805
ES 2237942	T3	20050801	ES 1999-948005	19990805
IN 2001MN00121	A	20050304	IN 2001-MN121	20010202
PRIORITY APPLN. INFO.:			US 1998-130214 A	19980806

	US 1997-37517P	P	19970210
	US 1997-55153P	P	19970808
	US 1998-20231	B2	19980206
	EP 1999-948005	A	19990805
	WO 1999-SE1339	W	19990805

OTHER SOURCE(S): CASREACT 132:137669; MARPAT 132:137669

GI



I

AB Novel intermediates and improvements in the synthesis of acyclic guanine nucleoside prodrugs I (R = Br, iodo, alkoxy; R1 = H, acyl; R2 = alkyl; R3R4 = (CH2)n; n = 2-4) (for example valtamociclovir stearate), including purine salts amenable to one pot alkylation with the acyclic side chain, acyclic 2-amino-6-halo-purine and protected guanine precursors, one pot manipulations thereof and last step work up procedures. Thus, (R)-2-amino-6-benzyloxy-7-(2-acetoxymethyl-4,4-diethoxybutyl)purine was prepd.via alkylation of 2-amino-6-benzyloxypurine with (2S)-2-acetoxymethyl-4,4-diethoxybutyl toluenesulfonate.

IC ICM C07D473-18
ICS C07D473-32; C07D473-00; C07C309-45

CC 33-9 (Carbohydrates)

IT 151370-28-4P 151370-33-1P 195156-77-5P 195157-18-7P 195157-23-4P
195157-25-6P 195157-27-8P 211374-33-3P 256949-13-0P 256949-17-4P
256949-19-6P 256949-20-9P 256949-27-6P ***256949-28-7P***
256949-29-8P 256949-30-1P 256949-31-2P 256949-32-3P
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(synthesis of acyclic nucleoside derivs. via alkylation reaction)

IT 10084-80-7P, N-(Benzyloxycarbonyl)valine anhydride 19690-23-4P
19916-73-5P 161118-67-8P 211374-36-6P 211374-37-7P
211374-38-8P 256949-16-3P 256949-18-5P 256949-21-0P 256949-22-1P
256949-23-2P 256949-24-3P 256949-25-4P 256949-26-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis of acyclic nucleoside derivs. via alkylation reaction)

IT ***256949-28-7P***
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(synthesis of acyclic nucleoside derivs. via alkylation reaction)

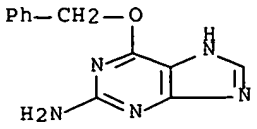
RN 256949-28-7 CAPLUS

CN 1H-Purin-2-amine, 6-(phenylmethoxy)-, compd. with 2,3,4,6,7,8,9,10-octahydropyrimido[1,2-a]azepine (1:1) (9CI) (CA INDEX NAME)

CM 1

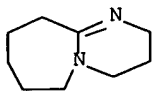
CRN 19916-73-5

CMF C12 H11 N5 O

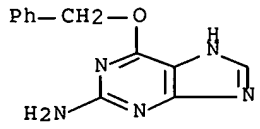


CM 2

CRN 6674-22-2
CMF C9 H16 N2



IT ***19916-73-5P***
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis of acyclic nucleoside derivs. via alkylation reaction)
RN 19916-73-5 CAPLUS
CN 9H-Purin-2-amine, 6-(phenylmethoxy)- (CA INDEX NAME)



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 5 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1999:46658 CAPLUS Full-text
DOCUMENT NUMBER: 131:73905
TITLE: A Practical Asymmetric Synthesis of the Antiviral Agent Lobucavir, BMS-180194. [Erratum to document cited in CA130:4011]
AUTHOR(S): Singh, Janak; Bisacchi, Gregory S.; Ahmad, Saleem; Godfrey, Jollie D., Jr.; Kissick, Thomas P.; Mitt, Toomas; Kocy, Octavian; Vu, Truc; Papaioannou, Chris G.; Wong, Michael K.; Heikes, James E.; Zahler, Robert; Mueller, Richard H.
CORPORATE SOURCE: The Bristol-Myers Squibb Pharmaceutical Research Institute, Princeton, NJ, 08543-4000, USA
SOURCE: Organic Process Research & Development (1999), 3(3), 235

CODEN: OPRDFK; ISSN: 1083-6160
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The structure of Feist's acid in Scheme 3 is incorrect. The correct structure is i in footnote 25 of this paper.

CC 33-9 (Carbohydrates)
Section cross-reference(s): 1

IT 19690-23-4P 132294-16-7P 132294-17-8P 132294-19-0P 138514-37-1P
138736-91-1P 138736-92-2P 138736-93-3P 156126-47-5P 156126-48-6P
156126-50-0P 156126-51-1P 156126-52-2P 156126-83-9P
163928-90-3P 163928-93-6P 163928-95-8P 163928-96-9P
215730-69-1P 215730-70-4P 215730-71-5P 215730-72-6P 215730-73-7P
215730-75-9P 215730-76-0P 215730-77-1P 215730-78-2P 215730-79-3P
215730-83-9P 215730-84-0P
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(practical asym. synthesis of antiviral agent lobucavir via asym. cycloaddn. of dimenthyl fumarate with ketene di-Me acetal (Erratum))

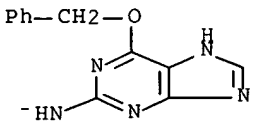
IT ***163928-90-3P***
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(practical asym. synthesis of antiviral agent lobucavir via asym. cycloaddn. of dimenthyl fumarate with ketene di-Me acetal (Erratum))

RN 163928-90-3 CAPLUS

CN 1-Butanaminium, N,N,N-tributyl-, salt with 6-(phenylmethoxy)-1H-purin-2-amine (1:1) (9CI) (CA INDEX NAME)

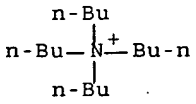
CM 1

CRN 163928-89-0
CMF C12 H10 N5 O



CM 2

CRN 10549-76-5
CMF C16 H36 N



L14 ANSWER 6 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1998:636366 CAPLUS Full-text
DOCUMENT NUMBER: 130:4011
TITLE: A Practical Asymmetric Synthesis of the Antiviral Agent Lobucavir, BMS-180194
AUTHOR(S): Singh, Janak; Bisacchi, Gregory S.; Ahmad, Saleem; Godfrey, Jollie D., Jr.; Kissick, Thomas P.; Mitt, Toomas; Kocy, Octavian; Vu, Truc; Papaioannou, Chris G.; Wong, Michael K.; Heikes, James E.; Zahler, Robert; Mueller, Richard H.
CORPORATE SOURCE: The Bristol-Myers Squibb Pharmaceutical Research Institute, Princeton, NJ, 08543-4000, USA
SOURCE: Organic Process Research & Development (1998), 2(6), 393-399
CODEN: OPRDFK; ISSN: 1083-6160
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 130:4011
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB A practical synthesis of the antiviral agent lobucavir, [1R-(1α,2β,3α)]-2-amino-9-[2,3-bis(hydroxymethyl)cyclobutyl]-6H-purin-6-one (BMS-180194) (I), is described. The key chiral intermediate, [1S-(1α,2β,3α)]- 3-hydroxy-1,2-cyclobutanedimethanol dibenzoate ester (II), was made by an asym. [2 + 2] cycloaddn. of dimenthyl fumarate with ketene di-Me acetal followed by sequential diester reduction, benzoylation, deketalization, and stereoselective ketone reduction Regioselective N9-alkylation of the tetra-n-butylammonium salt of 2-amino-6-iodopurine with the derived cyclobutyltriflate furnished the purinecyclobutyl dibenzoate (III). Methanolysis followed by acid hydrolysis produced lobucavir in a 35% overall yield with an ee > 99%.

CC 33-9 (Carbohydrates)
Section cross-reference(s): 1

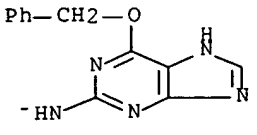
IT 19690-23-4P 132294-16-7P 132294-17-8P 132294-19-0P 138514-37-1P
138736-91-1P 138736-92-2P 138736-93-3P 156126-47-5P 156126-48-6P
156126-50-0P 156126-51-1P 156126-52-2P 156126-83-9P
163928-90-3P 163928-93-6P 163928-95-8P 163928-96-9P
215730-69-1P 215730-70-4P 215730-71-5P 215730-72-6P 215730-73-7P
215730-75-9P 215730-76-0P 215730-77-1P 215730-78-2P 215730-79-3P
215730-83-9P 215730-84-0P
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(practical asym. synthesis of antiviral agent lobucavir via asym. cycloaddn. of dimenthyl fumarate with ketene di-Me acetal)

IT ***163928-90-3P***
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(practical asym. synthesis of antiviral agent lobucavir via asym. cycloaddn. of dimenthyl fumarate with ketene di-Me acetal)

RN 163928-90-3 CAPLUS
CN 1-Butanaminium, N,N,N-tributyl-, salt with 6-(phenylmethoxy)-1H-purin-2-amine (1:1) (9CI) (CA INDEX NAME)

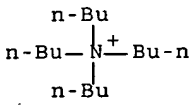
CM 1

CRN 163928-89-0
CMF C12 H10 N5 O



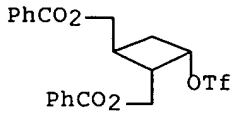
CM 2

CRN 10549-76-5
CMF C16 H36 N



REFERENCE COUNT: 52 THERE ARE 52 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1995:520756 CAPLUS Full-text
DOCUMENT NUMBER: 123:33570
TITLE: Regioselective Coupling of Tetraalkylammonium Salts of 6-Iodo-2-aminopurine to a Cyclobutyl Triflate: Efficient Preparation of Homochiral BMS-180,194, a Potent Antiviral Carbocyclic Nucleoside
AUTHOR(S): Bisacchi, Gregory S.; Singh, Janak; Godfrey, Jollie D., Jr.; Kissick, Thomas P.; Mitt, Toomas; Malley, Mary F.; Di Marco, John D.; Gougoutas, Jack Z.; Mueller, Richard H.; Zahler, Robert
CORPORATE SOURCE: Bristol-Myers Squibb Pharmaceutical Research Institute, Princeton, NJ, 08543, USA
SOURCE: Journal of Organic Chemistry (1995), 60(9), 2902-5
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 123:33570
GI



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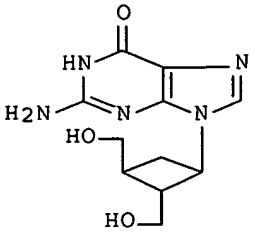


II

AB Tetra-N-alkylammonium salts of 6-iodo-2-aminopurine and several other 6-substituted-2-aminopurines were prepared by treating the purines with aqueous tetraalkylammonium hydroxide followed by removal of water. We studied the alkylation of several of these salts with acetivated cyclobutyl substrates. In particular, the tetra-N-butylammonium salt of 6-iodo-2-aminopurine reacted smoothly with an equimolar quantity of the cyclobutyl triflate I at room temperature in CH2Cl2 to provide the N-9 coupled nucleoside analog intermediate which was converted to carbocyclic nucleoside II in good yield. The excellent regioselectivity, high isolated yield of the N-9 isomer, and mild reaction conditions is remarkable for the alkylation of a guanine synthon with an activated carbocycle.

CC 33-9 (Carbohydrates)

IT 10310-21-1 132294-18-9 156126-50-0 156126-52-2 ***163928-90-3*** 163928-92-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(regioselective coupling of tetraalkylammonium salts of iodoaminopurine to a cyclobutyl triflate in preparation of homochiral potent antiviral carbocyclic nucleoside)

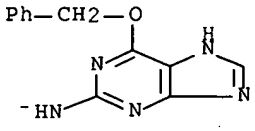
IT ***163928-90-3***
RL: RCT (Reactant); RACT (Reactant or reagent)
(regioselective coupling of tetraalkylammonium salts of iodoaminopurine to a cyclobutyl triflate in preparation of homochiral potent antiviral carbocyclic nucleoside)

RN 163928-90-3 CAPLUS

CN 1-Butanaminium, N,N,N-tributyl-, salt with 6-(phenylmethoxy)-1H-purin-2-amine (1:1) (9CI) (CA INDEX NAME)

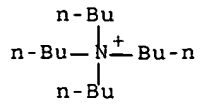
CM 1

CRN 163928-89-0
CMF C12 H10 N5 O

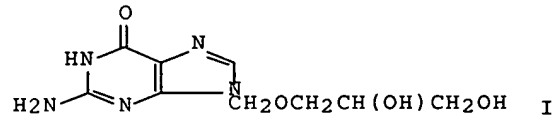


CM 2

CRN 10549-76-5
CMF C16 H36 N



L14 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1986:179770 CAPLUS Full-text
DOCUMENT NUMBER: 104:179770
TITLE: Enzymatic phosphorylation of the antiherpetic agent 9-[(2,3-dihydroxy-1-propoxy)methyl]guanine
AUTHOR(S): Karkas, J. D.; Ashton, W. T.; Canning, L. F.; Liou, R.; Germershausen, J.; Bostedor, R.; Arison, B.; Field, A. K.; Tolman, R. L.
CORPORATE SOURCE: Merck Sharp and Dohme Res. Lab., Rahway, NJ, 07065, USA
SOURCE: Journal of Medicinal Chemistry (1986), 29(5), 842-8
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



AB The antiherpetic agent (±)-9-[(2,3-dihydroxy-1-propoxy)methyl]guanine (I) [96429-66-2] is phosphorylated by herpes simplex virus-1 (HSV1) thymidine kinase, and its phosphorylated products inhibit DNA polymerase [9012-90-2] activity. I exists in two enantiomeric forms, each with a primary and a secondary hydroxyl; thus, a number of possibilities for preferential phosphorylation exist, which were explored in this study. HSV1 thymidine kinase [9002-06-6] phosphorylates the primary OH of both (R)-I [96480-02-3] and (S)-I [96480-03-4]. This was established by comparison with analogs in which either the primary or the secondary OH was replaced by F or H and also by a study of the NMR spectrum of the monophosphate. GMP kinase [9026-59-9] phosphorylates the monophosphates of R- and S-isomers to the resp. diphosphates. Further phosphorylation, however, is much more efficient with the S than with the R isomer. Furthermore, (S)-I triphosphate [100995-12-8] is a more potent inhibitor of HSV1 DNA polymerase than (R)-I triphosphate [100995-13-9]. These differences in the biochem. specificities of the 2 isomers account for the observed higher antiviral potency of (S)-I as compared to that of (R)-I.

CC 1-5 (Pharmacology)
Section cross-reference(s): 28

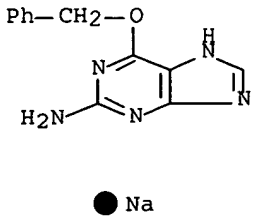
IT ***100994-97-6***

RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with (benzyloxy)(chloromethoxy)propane or -fluoropropane)

IT *100994-97-6*
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with (benzyloxy)(chloromethoxy)propane or -fluoropropane)

RN 100994-97-6 CAPLUS

CN 1H-Purin-2-amine, 6-(phenylmethoxy)-, monosodium salt (9CI) (CA INDEX NAME)



L14 ANSWER 9 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1982:582809 CAPLUS Full-text

DOCUMENT NUMBER: 97:182809

TITLE: Guanine derivatives

INVENTOR(S): Hagberg, Curt Erik; Johansson, Karl Nils Gunnar; Kovacs, Zsuzsanna Maria Ilona; Stening, Goeran Bertil

PATENT ASSIGNEE(S): Astra Lakemedel AB, Swed.

SOURCE: Eur. Pat. Appl., 74 pp.
CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

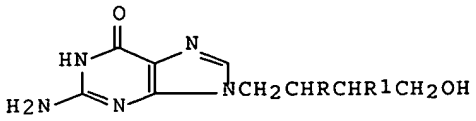
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 55239	A1	19820630	EP 1981-850250	19811222
EP 55239	B1	19860716		
R: AT, BE, CH, DE, FR, GB, IT, LU, NL, SE				
IL 64501	A	19850731	IL 1981-64501	19811210
ZA 8108781	A	19821124	ZA 1981-8781	19811218
AU 8178721	A	19820701	AU 1981-78721	19811221
AU 542373	B2	19850221		
CA 1172633	A1	19840814	CA 1981-392782	19811221
WO 8202202	A1	19820708	WO 1981-SE389	19811222
W: AU, DK, FI, HU, JP, NO, RO, SU				
AU 8279384	A	19820720	AU 1982-79384	19811222
JP 57501963	T	19821104	JP 1982-500239	19811222
HU 26700	A2	19830928	HU 1982-226	19811222
HU 190787	B	19861128		
AT 20748	T	19860815	AT 1981-850250	19811222
NO 8202712	A	19820809	NO 1982-2712	19820809
DK 8203699	A	19820818	DK 1982-3699	19820818
DK 148279	B	19850528		
DK 148279	C	19860217		
FI 8202891	A	19820819	FI 1982-2891	19820819
FI 68054	B	19850329		

FI 68054	C	19850710			
SU 1272991	A3	19861123	SU 1982-3480213		19820820
RO 85288	A1	19841125	RO 1982-108498		19820821
SU 1272992	A3	19861123	SU 1983-3657074		19831031
ES 550016	A3	19860401	ES 1985-550016		19851217
ES 550017	A3	19860401	ES 1985-550017		19851217
PRIORITY APPLN. INFO.:			SE 1980-9040	A	19801222
			EP 1981-850250	A	19811222
			WO 1981-SE389	A	19811222

OTHER SOURCE(S): MARPAT 97:182809

GI



I

AB Guanine derivs. I (R, R1 = H, OH, F), with antiviral activity, were prepared Thus, Et 4-(2-amino-6-chloropurin-9-yl)-2-hydroxybutyrate, prepared by the alkylation of 2-amino-6-chloropurine with BrCH2CH2CH(OH)CO2Et, was refluxed with 1M aqueous HCl to give 4-(2-amino-1,6-dihydro-6-oxopurin-9-yl)-2-hydroxybutyric acid, which was converted into its Et ester and then reduced with NaBH4 to give I (R = H, R1 = OH) (II). II at 5 μM concentration inhibited the herpes simplex type 1 plaque on vero cell monolayers by >90%.

IC C07D473-18; A61K031-52

CC 33-9 (Carbohydrates)
Section cross-reference(s): 1, 28, 63

IT ***83470-63-7P***
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with butanetriol derivative)

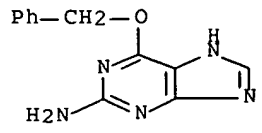
IT ***83470-63-7P***
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with butanetriol derivative)

RN 83470-63-7 CAPLUS

CN 1-Butanaminium, N,N,N-tributyl-, compd. with 6-(phenylmethoxy)-1H-purin-2-amine (1:1) (9CI) (CA INDEX NAME)

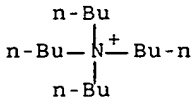
CM 1

CRN 19916-73-5
CMF C12 H11 N5 O



CM 2

CRN 10549-76-5
CMF C16 H36 N



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FILE COVERS 1907 - 9 Mar 2007 VOL 146 ISS 12
FILE LAST UPDATED: 8 Mar 2007 (20070308/ED)

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They are available for your review at:

http://www.cas.org/infopolicy.html
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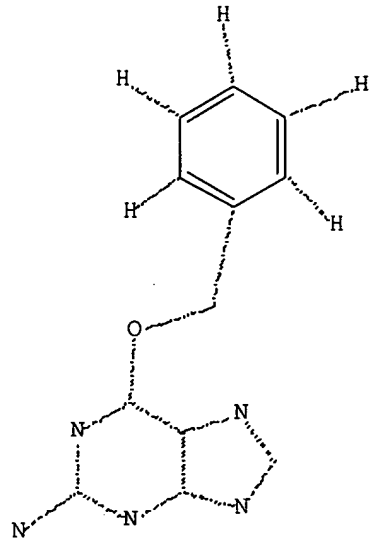

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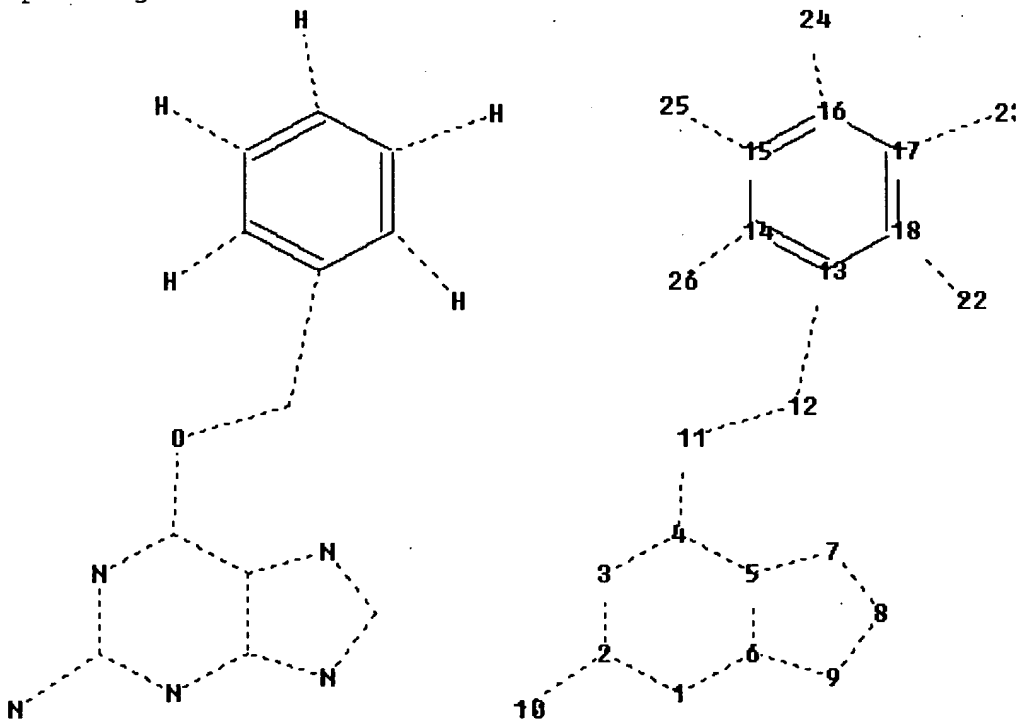

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ring nodes :
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chain bonds :
2-10 4-11 11-12 12-13 14-26 15-25 16-24 17-23 18-22
ring bonds :
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17-18
exact/norm bonds :
1-2 1-6 2-3 2-10 3-4 4-5 4-11 5-6 5-7 6-9 7-8 8-9 11-12 12-13 14-26
15-25 16-24 17-23 18-22
normalized bonds :
13-14 13-18 14-15 15-16 16-17 17-18

Connectivity :
1:2 E exact RC ring/chain 2:3 E exact RC ring/chain 3:2 E exact RC ring/chain
4:3 E exact RC ring/chain 5:3 E exact RC ring/chain 6:3 E exact RC ring/chain
7:2 E exact RC ring/chain
8:2 E exact RC ring/chain 9:2 E exact RC ring/chain 10:1 E exact RC ring/chain
11:2 E exact
RC ring/chain 12:2 E exact RC ring/chain 13:3 E exact RC ring/chain
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:CLASS 12:CLASS 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 22:CLASS
23:CLASS 24:CLASS
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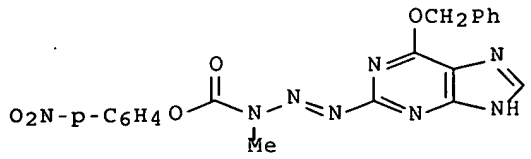
L18 ANSWER 1 OF 41 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:1005649 CAPLUS Full-text
DOCUMENT NUMBER: 142:134353
TITLE: Synthesis and Antitumor Activity of Methyltriazene Prodrugs Simultaneously Releasing DNA-Methylating Agents and the Antiresistance Drug O6-Benzylguanine
AUTHOR(S): Wanner, Martin J.; Koch, Melle; Koomen, Gerrit-Jan
CORPORATE SOURCE: Laboratory of Bioorganic Chemistry, Van't Hoff Institute of Molecular Sciences, University of Amsterdam, Amsterdam, NL-1018 WS, Neth.
SOURCE: Journal of Medicinal Chemistry (2004), 47(27), 6875-6883
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 142:134353
GI



I

AB Active resistance of tumor cells against DNA alkylating agents arises by the production of high levels of the DNA repair protein O6-alkylguanine-DNA alkyltransferase (AGT). This resistance during treatment with, for example, the anticancer agent temozolomide can be reversed by administration of O6-benzylguanine, a purine that transfers its benzyl group to AGT and irreversibly inactivates it. Stimulated by the favorable therapeutic properties of temozolomide we designed and synthesized DNA-methylating triazenes built on the antiresistance benzylguanine ring system. The condensation reaction between 2-nitrosopurines and acylhydrazines proved to be very suitable to prepare acylated methyltriazenes. Fine-tuning of the release rate of both the methylating agent (diazomethane) and of O6-benzylguanine was accomplished by variation of the hydrolysis-sensitive acyl substituent. Hydrolysis studies were performed with 1H NMR and revealed that the p-nitrophenyl substituted triazene I showed an optimal hydrolysis rate (t1/2 = 23 min) and almost 100% selectivity for the desired fragmentation route. In vitro antitumor studies in the 60 human tumor cell line panel of the National Cancer Institute confirmed the superior properties of p-nitrophenyl-protected Me triazene I, showing mean IC50 values of 10 μM compared to 100 μM for temozolomide. In analogy with temozolomide, triazene I showed however low preference for each of the cancer subpanels, with IC50 values between 8 and 14 μM.

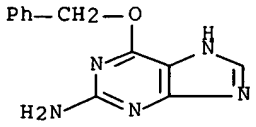
CC 26-9 (Biomolecules and Their Synthetic Analogs)
Section cross-reference(s): 1, 22

IT ***19916-73-5P***, O6-Benzylguanine 160948-25-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis, hydrolysis and antitumor activity of methyltriazene benzylguanine prodrugs)

IT ***19916-73-5P***, O6-Benzylguanine
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis, hydrolysis and antitumor activity of methyltriazene benzylguanine prodrugs)

RN 19916-73-5 CAPLUS

CN 9H-Purin-2-amine, 6-(phenylmethoxy)- (CA INDEX NAME)



REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 2 OF 41 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:748377 CAPLUS Full-text

DOCUMENT NUMBER: 141:366076

TITLE: Synthesis of 6-O-benzylguanine and its conjugations with linkers

AUTHOR(S): Barth, Claudia; Seitz, Oliver; Kunz, Horst

CORPORATE SOURCE: Institut fur Organische Chemie, Johannes Gutenberg-Universitaet Mainz, Mainz, D-55128, Germany

SOURCE: Zeitschrift fuer Naturforschung, B: Chemical Sciences (2004), 59(7), 802-806

CODEN: ZNBSEN; ISSN: 0932-0776
PUBLISHER: Verlag der Zeitschrift fuer Naturforschung
DOCUMENT TYPE: Journal
LANGUAGE: German
OTHER SOURCE(S): CASREACT 141:366076

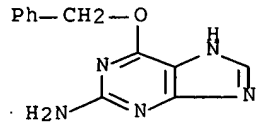
AB An improved synthesis of 6-O-benzyl guanine which is an important inhibitor of O6-alkyl-guanine DNA alkyltransferase is described. In addition the conjugation of this guanine derivative was, achieved with a functionalized hydrophilic linker which is of interest for immobilization of this inhibitor and its conjugation with targeting components.

CC 26-9 (Biomolecules and Their Synthetic Analogs)
Section cross-reference(s): 1, 28

IT ***19916-73-5P*** 133803-81-3P 780761-84-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 6-O-benzylguanine and its conjugations with linkers)

IT ***19916-73-5P***
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 6-O-benzylguanine and its conjugations with linkers)

RN 19916-73-5 CAPLUS
CN 9H-Purin-2-amine, 6-(phenylmethoxy)- (CA INDEX NAME)

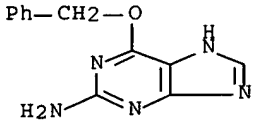


REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 3 OF 41 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:362549 CAPLUS Full-text
DOCUMENT NUMBER: 141:136595
TITLE: Synthesis and characterization of bifunctional probes for the specific labeling of fusion proteins
AUTHOR(S): Kindermann, Maik; Sielaff, India; Johnsson, Kai
CORPORATE SOURCE: Institute of Chemical Sciences and Engineering, Ecole Polytechnique Federale de Lausanne, Lausanne, CH-1015, Switz.
SOURCE: Bioorganic & Medicinal Chemistry Letters (2004), 14(11), 2725-2728
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 141:136595

AB Labeling proteins with synthetic probes is important for studying and characterizing protein function. We have recently introduced a general method for the specific in vivo and in vitro labeling of fusion proteins that is based on the reaction of O6-alkylguanine-DNA alkyltransferase (AGT) with O6-benzylguanine derivs. Here we report two complementary routes for the synthesis of O6-benzylguanine derivs., which allow for the labeling of AGT fusion proteins with bifunctional synthetic probes and demonstrate the specific labeling of AGT fusion proteins with these probes. These mols. should become useful tools for various applications in functional proteomics.

CC 9-16 (Biochemical Methods)
Section cross-reference(s): 7
IT ***19916-73-5DP***, O6-Benzylguanine, derivs. 680622-86-0P
680622-87-1P 725747-36-4P
RL: ARU (Analytical role, unclassified); BUU (Biological use, unclassified); RCT (Reactant); SPN (Synthetic preparation); ANST (Analytical study); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(synthesis and characterization of bifunctional probes for specific labeling of fusion proteins)
IT ***19916-73-5DP***, O6-Benzylguanine, derivs.
RL: ARU (Analytical role, unclassified); BUU (Biological use, unclassified); RCT (Reactant); SPN (Synthetic preparation); ANST (Analytical study); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(synthesis and characterization of bifunctional probes for specific labeling of fusion proteins)
RN 19916-73-5 CAPLUS
CN 9H-Purin-2-amine, 6-(phenylmethoxy)- (CA INDEX NAME)



REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 4 OF 41 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:264590 CAPLUS Full-text
DOCUMENT NUMBER: 140:304080
TITLE: Solid-phase synthesis of peptide nucleic acids and their DNA-binding properties
INVENTOR(S): Buchardt, Ole; Egholm, Michael; Nielsen, Peter Eigil; Berg, Rolf Henrik
PATENT ASSIGNEE(S): Den.
SOURCE: U.S., 91 pp., Cont.-in-part of U.S. Ser. No. 108,591.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 19
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6713602	B1	20040330	US 1995-462977	19950605
CA 2109320	A1	19921125	CA 1992-2109320	19920522
CA 2109320	C	20030722		
AU 9218806	A	19921230	AU 1992-18806	19920522
AU 666480	B2	19960215		
EP 586618	A1	19940316	EP 1992-923579	19920522
EP 586618	B1	19970716		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
JP 06509063	T	19941013	JP 1992-510139	19920522
EP 1074559	A1	20010207	EP 2000-203148	19920522
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC				

EP 1162206	A2	20011212	EP 2001-203303	19920522
EP 1162206	A3	20040414		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC				
JP 2003235590	A	20030826	JP 2003-15384	19920522
EP 1411063	A1	20040421	EP 2003-77836	19920522
EP 1411063	B1	20060719		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC				
US 6395474	B1	20020528	US 1993-108591	19931122
NO 9304235	A	19940120	NO 1993-4235	19931123
NO 313201	B1	20020826		
US 6357163	B1	20020319	US 1994-150156	19940504
US 5773571	A	19980630	US 1996-595387	19960201
US 2002160383	A1	20021031	US 2001-983210	20011023
US 2003180734	A1	20030925	US 2002-154890	20020523
US 2006160731	A1	20060720	US 2003-691012	20031022
US 2005009041	A1	20050113	US 2004-755118	20040109
US 2006046255	A1	20060302	US 2005-29005	20050105

PRIORITY APPLN. INFO.:

DK 1991-986	A	19910524
DK 1991-987	A	19910524
DK 1992-510	A	19920415
US 1993-108591	A2	19931122
EP 1992-911165	A3	19920522
EP 2000-203148	A3	19920522
JP 1992-510139	A3	19920522
WO 1992-EP1219	W	19920522
WO 1992-EP1220	A	19920522
US 1993-54363	A3	19930426
US 1994-150156	A1	19940504
US 1995-462977	A1	19950605
US 2001-983210	B1	20011023
US 2002-154890	A3	20020523

OTHER SOURCE(S): MARPAT 140:304080

AB A novel class of compds., known as peptide nucleic acids (PNAs), bind complementary ssDNA and RNA strands more strongly than a corresponding DNA and generally comprise ligands such as naturally occurring DNA bases attached to a peptide backbone through a suitable linker. In certain embodiments, the PNAs have formula Q-T1-B1(-A1-L1)-D1-G1-T2-B2(-A2-L2)-D2- G2-Tn-Bn(-An-Ln)-Dn-I [n ≥ 2; each L1-Ln is H, OH, alkanoyl, naturally or non-naturally occurring nucleobases, aromatic moieties, DNA intercalators, nucleobase-binding groups, heterocyclic moieties, and reporter ligands; each A1-An is a single bond, CH2, (un)substituted (hetero)alkylene; each B1-Bn is N or R3N+, where R3 is H, alkyl, OH, amino, etc.; each of T1-Tn is CR6R7, CHR6CHR7 or CR6R7CH2, where R6 is H and R7 is a side chain of a naturally occurring α-amino acid or R6, R7 are H, alkyl, aryl, (hetero)aryl, etc.; each D1-Dn is CR6R7, CH2CR6R7 or CHR6CHR7; each G1-Gn is NR3CO, NR3CS, NR3SO, or NR3SO2; Q is CO2H or SO3H or an activated derivative, a carbamoyl or sulfamoyl group; I is an amino or acylamino group]. Solid-phase methods are described for the synthesis of the PNAs, e.g., H-[Taeg]4-[Caeg]2-Taeg-Caeg-Taeg-Caeg-Lys-NH2 (aeg is an aminoethyglycine residue, T and C are thymine and cytosine residues; also denoted H-T4-C2TCTC-Lys-NH2), for which hybridization data are tabulated. The examples also give biochem./biol. properties of PNA oligomers, including: sequence discrimination at the dsDNA level, kinetics of PNA-T10-dsDNA strand displacement complex formation, stability of a PNA-dsDNA complex, inhibition of restriction enzyme cleavage by PNA, and binding of 125I-labeled PNA to oligonucleotides.

IC ICM A61K038-00
ICS C07K001-00; C12Q001-68; C07H021-00

INCL 530300000; 435006000; 530350000; 536023100

CC 34-3 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 6, 33

IT 4113-97-7P 5236-60-2P 6214-59-1P ***19916-73-5P*** 25477-96-7P
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144564-94-3P 144564-95-4P 149035-00-7P 149035-01-8P 149035-02-9P
149035-03-0P 149376-49-8P 149376-50-1P 149376-51-2P 149376-63-6P
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149376-71-6P 149376-72-7P 149376-73-8P 149376-74-9P 149376-76-1P
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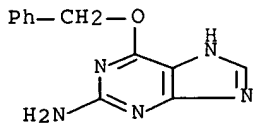
171855-80-4P 183727-86-8P 183727-87-9P 202999-51-7P 202999-52-8P
676241-23-9P 676241-24-0P 676241-25-1P 676241-26-2P 676241-27-3P
676241-28-4P 676241-29-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(solid-phase synthesis of peptide nucleic acids and their DNA-binding properties)

IT ***19916-73-5P***
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(solid-phase synthesis of peptide nucleic acids and their DNA-binding properties)

RN 19916-73-5 CAPLUS
CN 9H-Purin-2-amine, 6-(phenylmethoxy)- (CA INDEX NAME)



REFERENCE COUNT: 240 THERE ARE 240 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 5 OF 41 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:240415 CAPLUS Full-text
DOCUMENT NUMBER: 140:287714
TITLE: Peptide nucleic acids with Nα-(2-aminoethyl)-histidine backbones having enhanced binding affinity and sequence specificity
INVENTOR(S): Nielsen, Peter E.; Egholm, Michael; Berg, Rolf H.; Buchardt, Ole
PATENT ASSIGNEE(S): Den.
SOURCE: U.S., 70 pp., Cont.-in-part of U.S. 5,719,262.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 19
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6710164	B1	20040323	US 1999-230088	19990310

US 6395474	B1	20020528	US 1993-108591		19931122
US 5773571	A	19980630	US 1996-595387		19960201
US 5714331	A	19980203	US 1996-686116		19960724
US 5719262	A	19980217	US 1996-685484		19960724
US 5766855	A	19980616	US 1996-686113		19960724
US 6414112	B1	20020702	US 1996-686114		19960724
WO 9803542	A1	19980129	WO 1997-US12811		19970724

W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AN

RW: GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG

US 6107470	A	20000822	US 1999-225146		19990104
US 2006160731	A1	20060720	US 2003-691012		20031022

PRIORITY APPLN. INFO.:

US 1993-108591	A2	19931122
US 1996-685484	A2	19960724
US 1996-686113	A2	19960724
US 1996-686114	A2	19960724
US 1996-686116	A2	19960724
US 1997-51002P	P	19970529
WO 1997-US12811	W	19970724
DK 1991-986	A	19910524
DK 1991-987	A	19910524
DK 1992-510	A	19920415
WO 1992-EP1219	W	19920522
US 1993-54363	A3	19930426
US 1998-69705	A1	19980429
US 2002-154890	A3	20020523

OTHER SOURCE(S): MARPAT 140:287714

AB Peptide nucleic acid (PNA) monomers comprising Nα-(2-aminoethyl)-(D or L)-His-OH backbones as well as various derivs. of these monomers are disclosed. Replacement of Gly in the classical PNA backbone with His may enhance sequence specificity, binding affinity, and/or solubility of the PNA.

IC ICM A61K038-00
ICS C12Q001-68; G01N033-566

INCL 530300000; 435006000; 436501000

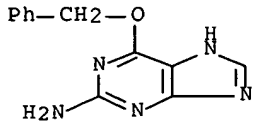
CC 34-3 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 1, 6, 26

IT 4113-97-7P 5236-60-2P 6214-59-1P 13303-10-1P, tert-Butyl p-nitrophenyl carbonate ***19916-73-5P*** 20924-05-4P, 1-(Carboxymethyl)thymine 25477-96-7P 31385-63-4P 34046-07-6P 57260-73-8P 72648-80-7P 84891-29-2P 85301-38-8P 85301-50-4P 89459-22-3P 90495-99-1P 128421-86-3P 137618-48-5P 139166-79-3P 139166-80-6P 139166-81-7P 139166-82-8P 139924-84-8P 144564-94-3P 144564-95-4P 149035-00-7P 149035-01-8P 149035-02-9P 149035-03-0P 149376-49-8P 149376-50-1P 149376-51-2P 149376-66-9P 149376-67-0P 149376-68-1P 149376-69-2P 149376-70-5P 149376-71-6P 149376-72-7P 149376-73-8P 149376-74-9P 149376-76-1P 149376-78-3P 149376-79-4P 149376-80-7P 149376-81-8P 149376-82-9P 149376-83-0P 149411-91-6P 149411-92-7P 149411-93-8P 149411-94-9P 149465-96-3P 149465-97-4P 149465-98-5P 149494-90-6P 149500-73-2P 149500-74-3P 163081-00-3P 163081-01-4P 163081-06-9P 202343-70-2P 202343-71-3P 202999-28-8P 202999-51-7P 202999-52-8P 209331-73-7P 209331-76-0P 209331-79-3P 209331-82-8P 209332-02-5P 209332-04-7P 209332-06-9P 209332-10-5P 209332-12-7P 675107-01-4P 675107-02-5P 675107-03-6P 675107-04-7P 675107-05-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)
(peptide nucleic acids with Nα-(2-aminoethyl)-histidine backbones having enhanced binding affinity and sequence specificity)

IT ***19916-73-5P***
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(peptide nucleic acids with Nα-(2-aminoethyl)-histidine backbones having enhanced binding affinity and sequence specificity)

RN 19916-73-5 CAPLUS
CN 9H-Purin-2-amine, 6-(phenylmethoxy)- (CA INDEX NAME)



REFERENCE COUNT: 167 THERE ARE 167 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 6 OF 41 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:205972 CAPLUS Full-text
DOCUMENT NUMBER: 142:176578
TITLE: Product class 17: purines
AUTHOR(S): Seela, F.; Ramzaeva, N.; Rosemeyer, H.
CORPORATE SOURCE: Germany
SOURCE: Science of Synthesis (2004), 16, 945-1108
CODEN: SSCYJ9
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English

AB A review. Methods for preparing purines are reviewed including cyclization, ring transformation, and substituent modification. Oxidation of purines is included.

CC 26-0 (Biomolecules and Their Synthetic Analogs)

IT 69-93-2P, preparation 146-78-1P 605-99-2P 612-37-3P 653-45-2P
700-00-5P 700-02-7P 708-79-2P 778-98-3P 875-31-0P 934-23-6P
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1598-61-4P 1660-91-9P, 1H-Purine-8-d 1681-15-8P 1839-18-5P
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153285-52-0P 155588-82-2P 155588-83-3P 155588-84-4P 155588-86-6P
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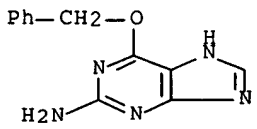
160516-14-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and oxidation of purines via cyclization, ring transformation and
substituent modification)

IT ***19916-73-5P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and oxidation of purines via cyclization, ring transformation and
substituent modification)

RN 19916-73-5 CAPLUS
CN 9H-Purin-2-amine, 6-(phenylmethoxy)- (CA INDEX NAME)



REFERENCE COUNT: 762 THERE ARE 762 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 7 OF 41 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:173561 CAPLUS Full-text
DOCUMENT NUMBER: 141:327951
TITLE: Labeling of fusion proteins of O6-alkylguanine-DNA alkyltransferase with small molecules in vivo and in vitro

AUTHOR(S): Keppler, Antje; Kindermann, Maik; Gendreizig, Susanne; Pick, Horst; Vogel, Horst; Johnsson, Kai

CORPORATE SOURCE: Institute of Molecular and Biological Chemistry, Ecole Polytechnique Federale de Lausanne (EPFL), Lausanne, CH-1015, Switz.

SOURCE: Methods (San Diego, CA, United States) (2004), 32(4), 437-444
CODEN: MTHDE9; ISSN: 1046-2023

PUBLISHER: Elsevier Science

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The in vivo and in vitro labeling of fusion proteins with synthetic mols. capable of probing and controlling protein function has the potential to become an important method in functional genomics and proteomics. We have recently introduced an approach for the specific labeling of fusion proteins, which is based on the generation of fusion proteins with the human DNA repair protein O6-alkylguanine-DNA alkyltransferase (hAGT) and the irreversible reaction of hAGT with O6-benzylguanine derivs. Here, we report optimized protocols for the synthesis of O6-benzylguanine derivs. and the use of such derivs. for the labeling of different hAGT fusion proteins in vivo and in vitro.

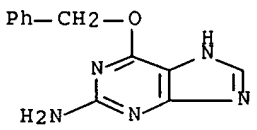
CC 9-14 (Biochemical Methods)
Section cross-reference(s): 7

IT ***19916-73-5DP***, O6-Benzylguanine, derivs.
RL: BUU (Biological use, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(protein label; labeling of fusion proteins of O6-alkylguanine-DNA alkyltransferase with O6-benzylguanine derivs. in vivo and in vitro)

IT ***19916-73-5DP***, O6-Benzylguanine, derivs.
RL: BUU (Biological use, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(protein label; labeling of fusion proteins of O6-alkylguanine-DNA alkyltransferase with O6-benzylguanine derivs. in vivo and in vitro)

RN 19916-73-5 CAPLUS

CN 9H-Purin-2-amine, 6-(phenylmethoxy)- (CA INDEX NAME)



REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 8 OF 41 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2003:512728 CAPLUS Full-text

DOCUMENT NUMBER: 140:218061

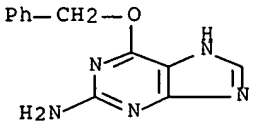
TITLE: Synthesis of new chiral building blocks for novel peptide nucleic acids

AUTHOR(S): Wu, Jie; Xu, Xiao-Yu; Liu, Ke-Liang

CORPORATE SOURCE: Beijing Institute of Pharmacology and Toxicology, Beijing, 100850, Peop. Rep. China

SOURCE: Chinese Journal of Chemistry (2003), 21(5), 566-573
CODEN: CJOCEV; ISSN: 1001-604X

PUBLISHER: Science Press
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 140:218061
AB Nucleic acid base-substituted N-protected proline derivs. were prepared as conformationally constrained chiral building blocks for peptide nucleic acids.
CC 34-3 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 33
IT 4330-20-5P ***19916-73-5P*** 627100-71-4P 663948-82-1P
663948-83-2P 663948-84-3P 663948-85-4P 663948-86-5P 663948-87-6P
663948-88-7P 663948-89-8P 663948-91-2P 663948-92-3P 663948-94-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of nucleic acid base-substituted N-protected proline derivs. as
chiral building blocks for peptide nucleic acids)
IT ***19916-73-5P***
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of nucleic acid base-substituted N-protected proline derivs. as
chiral building blocks for peptide nucleic acids)
RN 19916-73-5 CAPLUS
CN 9H-Purin-2-amine, 6-(phenylmethoxy)- (CA INDEX NAME)



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L18 ANSWER 9 OF 41 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:407910 CAPLUS Full-text
DOCUMENT NUMBER: 140:177369
TITLE: Synthesis and preliminary biological evaluation of radiolabeled O6-benzylguanine derivatives, new potential PET imaging agents for the DNA repair protein O6-alkylguanine-DNA alkyltransferase in breast cancer
AUTHOR(S): Zheng, Qi-Huang; Liu, Xuan; Fei, Xiangshu; Wang, Ji-Quan; Ohannesian, David W.; Erickson, Leonard C.; Stone, K. Lee; Hutchins, Gary D.
CORPORATE SOURCE: Department of Radiology, Indiana University School of Medicine, Indianapolis, IN, 46202, USA
SOURCE: Nuclear Medicine and Biology (2003), 30(4), 405-415
CODEN: NMBIEO; ISSN: 0969-8051
PUBLISHER: Elsevier Science Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Novel radiolabeled O6-benzylguanine (O6-BG) derivs., 2-amino-6-O-[11C]-[(methoxymethyl)benzyloxy]-9-Me purines ([11C]p-O6-AMMP); [11C]m-O6-AMMP; [11C]o-O6-AMMP, 2-amino-6-O-benzyloxy-9-[11C]- [(methoxycarbonyl)methyl]purine ([11C]ABMMP), and 2-amino-6-O-benzyloxy-9- [11C]-[(4'-methoxycarbonyl)benzyl]purine ([11C]ABMBP), have been synthesized for

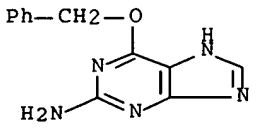
evaluation as new potential positron emission tomog. (PET) imaging agents for the DNA repair protein O6-alkylguanine-DNA alkyltransferase (AGT) in breast cancer. The appropriate precursors for radiolabeling were obtained in two to three steps from starting material 2-amino-6-chloropurine with moderate to excellent chemical yields. Tracers were prepared by O-[11C]methylation of hydroxymethyl or acid precursors using [11C]methyl triflate. Pure target compds. were isolated by solid-phase extraction (SPE) purification procedure in 45-65% radiochem. yields (decay corrected to end of bombardment), and a synthesis time of 20-25 min. The activity of unlabeled standard samples was evaluated via an in vitro AGT oligonucleotide assay. Preliminary findings from biol. assay indicate the synthesized analogs have similar strong inhibitory effectiveness on AGT in comparison with the parent compound O6-BG. The results warrant further evaluation of these radiotracers as new potential PET imaging agents for the DNA repair protein AGT in breast cancer in vivo.

CC 8-9 (Radiation Biochemistry)
Section cross-reference(s): 28

IT 3035-73-2P ***19916-73-5P*** 62172-88-7P 62172-89-8P
149376-70-5P 149411-94-9P 203202-58-8P 522622-95-3P 658699-59-3P
658699-60-6P 658699-61-7P 658699-62-8P 658699-63-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis and evaluation of radiolabeled O6-benzylguanine derivs. as PET imaging agents for alkylguanine-DNA alkyltransferase in breast cancer)

IT ***19916-73-5P***
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis and evaluation of radiolabeled O6-benzylguanine derivs. as PET imaging agents for alkylguanine-DNA alkyltransferase in breast cancer)

RN 19916-73-5 CAPLUS
CN 9H-Purin-2-amine, 6-(phenylmethoxy)- (CA INDEX NAME)



REFERENCE COUNT: 52 THERE ARE 52 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 10 OF 41 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:318755 CAPLUS Full-text
DOCUMENT NUMBER: 139:100965
TITLE: A convenient procedure for the synthesis of O6-benzylguanine derivatives by phase transfer catalysis
AUTHOR(S): Liu, Xuan; Zheng, Qi-Huang; Hutchins, Gary D.; Fei, Xiangshu; Erickson, Leonard C.; Miller, Kathy D.; Mock, Bruce H.; Glick-Wilson, Barbara E.; Winkle, Wendy L.; Stone, K. Lee; Carlson, Kathy A.
CORPORATE SOURCE: Department of Radiology, Indiana University School of Medicine, Indianapolis, IN, 46202-5121, USA
SOURCE: Synthetic Communications (2003), 33(6), 941-952
CODEN: SYNCAV; ISSN: 0039-7911
PUBLISHER: Marcel Dekker, Inc.

DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 139:100965

AB A convenient procedure by phase transfer catalysis has been developed for the synthesis of O6-benzylguanine and its derivs. hydroxymethyl-O6- benzylguanine, halo-O6-benzylguanine, methoxy-O6-benzylguanine, and methyl-O6-benzylguanine derivs.

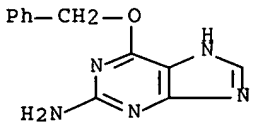
CC 26-9 (Biomolecules and Their Synthetic Analogs)

IT 100-51-6P, Benzyl alcohol, preparation 10310-21-1P, 2-Amino-6-chloropurine ***19916-73-5P*** 129409-64-9P 129409-65-0P
144084-37-7P 152832-91-2P 154010-52-3P 168098-94-0P 168098-95-1P
321195-47-5P 452973-13-6P 561014-68-4P 561014-69-5P 561014-70-8P
561014-71-9P 561014-72-0P 561014-73-1P 561014-74-2P 561014-75-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis of O6-benzylguanine derivs. by phase transfer catalysis)

IT ***19916-73-5P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis of O6-benzylguanine derivs. by phase transfer catalysis)

RN 19916-73-5 CAPLUS

CN 9H-Purin-2-amine, 6-(phenylmethoxy)- (CA INDEX NAME)



REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 11 OF 41 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:502839 CAPLUS Full-text
DOCUMENT NUMBER: 137:75059
TITLE: Peptide nucleic acids having 2,6-diaminopurine nucleobases and D-lysine in polyamide backbone
INVENTOR(S): Buchardt, Dorte; Egholm, Michael; Nielsen, Peter Eigil; Berg, Rolf Henrik
PATENT ASSIGNEE(S): Buchardt, Ole, Germany
SOURCE: U.S., 72 pp., Cont.-in-part of U.S. Ser. No. 108,591.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 19
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6414112	B1	20020702	US 1996-686114	19960724
CA 2109320	A1	19921125	CA 1992-2109320	19920522
CA 2109320	C	20030722		
AU 9218806	A	19921230	AU 1992-18806	19920522
AU 666480	B2	19960215		
EP 586618	A1	19940316	EP 1992-923579	19920522
EP 586618	B1	19970716		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
JP 06509063	T	19941013	JP 1992-510139	19920522
EP 1074559	A1	20010207	EP 2000-203148	19920522

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC

EP 1162206	A2	20011212	EP 2001-203303	19920522
EP 1162206	A3	20040414		

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC

JP 2003235590	A	20030826	JP 2003-15384	19920522
EP 1411063	A1	20040421	EP 2003-77836	19920522
EP 1411063	B1	20060719		

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US 6395474	B1	20020528	US 1993-108591	19931122
NO 9304235	A	19940120	NO 1993-4235	19931123
NO 313201	B1	20020826		
US 6357163	B1	20020319	US 1994-150156	19940504
US 5773571	A	19980630	US 1996-595387	19960201
CA 2261566	A1	19980129	CA 1997-2261566	19970724
WO 9803542	A1	19980129	WO 1997-US12811	19970724

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RW: GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG

AU 9738081	A	19980210	AU 1997-38081	19970724
AU 717387	B2	20000323		
EP 960121	A1	19991201	EP 1997-935053	19970724

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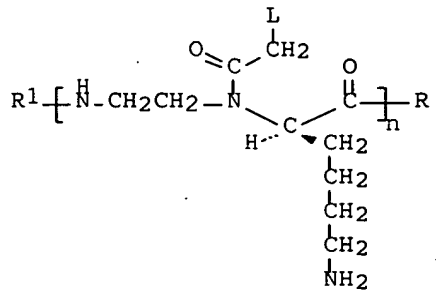
JP 2000503671	T	20000328	JP 1998-507186	19970724
JP 3306073	B2	20020724		
JP 2002105059	A	20020410	JP 2001-222248	19970724
AT 311402	T	20051215	AT 1997-935053	19970724
US 6710164	B1	20040323	US 1999-230088	19990310
US 6613873	B1	20030902	US 1999-337304	19990621
US 2002146718	A1	20021010	US 2001-955410	20010918
US 2002160383	A1	20021031	US 2001-983210	20011023
US 2003180734	A1	20030925	US 2002-154890	20020523
US 2006160731	A1	20060720	US 2003-691012	20031022
US 2006046255	A1	20060302	US 2005-29005	20050105

PRIORITY APPLN. INFO.:

DK 1991-986	A	19910524
DK 1991-987	A	19910524
DK 1992-510	A	19920415
US 1993-108591	A2	19931122
EP 1992-911165	A3	19920522
EP 2000-203148	A3	19920522
JP 1992-510139	A3	19920522
WO 1992-EP1219	W	19920522
WO 1992-EP1220	A	19920522
US 1993-54363	A3	19930426
US 1994-150156	A1	19940504
US 1996-685484	A	19960724
US 1996-686113	A	19960724
US 1996-686114	A	19960724
US 1996-686116	A	19960724
US 1997-847110	B1	19970501
US 1997-51002P	P	19970529
JP 1998-507186	A3	19970724
WO 1997-US12811	W	19970724
US 2001-983210	B1	20011023
US 2002-154890	A3	20020523

OTHER SOURCE(S): MARPAT 137:75059
GI



I

AB Peptide nucleic acids (PNAs) [I; L = naturally occurring or non-naturally occurring nucleobase with the proviso that at least one of L is 2,6-diaminopurine; R = OH, NH2, Lys-NH2; R1 = H, Ac, CO2CMe3 (Boc); n = 1-30] are disclosed. These PNAs bind complementary DNA and RNA strands more strongly than a corresponding DNA, and exhibit increased sequence specificity and solubility Thus, the Tm for PNA H-GTkAGATkCACTk-NH2 (II; aminoethylglycine backbone except where k appears, which is aminoethyl-D-lysine) binding to antiparallel complementary DNA was 55° while that for PNA H-GTAGATCACT-NH2 (III; with aminoethylglycine backbone) was 52°. The presence of the D-lysine also enhanced sequence specificity: in the presence of a single mismatch in the complementary DNA, the Tm's were 38° and 42° for II and III, resp. A 16-mer PNA containing four lysine side chains was soluble in physiol. useful solns. while the PNA devoid of the lysine side chains was insol. A 12-mer PNA containing two 2,6-diaminopurine nucleobases bearing lysine side chains, prepared by solid-phase methods using Nα-Boc and benzyl side chain protection, blocked in vitro translation of hepatitis C virus protein with EC50 = 29 nM.

IC ICM A61K038-00
ICS C07H021-00; C12Q001-68

INCL 530300000

CC 6-2 (General Biochemistry)
Section cross-reference(s): 1

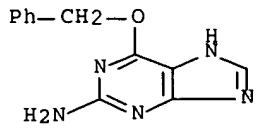
IT 4113-97-7P 5236-60-2P 6214-59-1P 13303-10-1P ***19916-73-5P***
20924-05-4P 25477-96-7P 31385-63-4P 57260-73-8P 70889-83-7P
85301-38-8P 89711-08-0P 90495-99-1P 137618-48-5P 139166-79-3P
139166-80-6P 139166-81-7P 139166-82-8P 139924-84-8P 144564-94-3P
144564-95-4P 149035-00-7P 149035-01-8P 149035-02-9P 149035-03-0P
149376-49-8P 149376-50-1P 149376-51-2P 149376-66-9P 149376-67-0P
149376-68-1P 149376-69-2P 149376-70-5P 149376-71-6P 149376-72-7P
149376-73-8P 149376-74-9P 149376-76-1P 149376-78-3P 149376-79-4P
149376-80-7P 149376-81-8P 149376-82-9P 149376-83-0P 149411-91-6P
149411-92-7P 149411-93-8P 149411-94-9P 149465-96-3P 149465-97-4P
149465-98-5P 149494-90-6P 149500-73-2P 149500-74-3P 163081-00-3P
163081-01-4P 163081-06-9P 202343-70-2P 202343-71-3P 202999-28-8P
202999-51-7P 202999-52-8P 209331-79-3P 209331-82-8P 439791-83-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(peptide nucleic acids having 2,6-diaminopurine nucleobases and D-lysine in polyamide backbone)

IT ***19916-73-5P***
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)
(peptide nucleic acids having 2,6-diaminopurine nucleobases and D-lysine in polyamide backbone)

RN 19916-73-5 CAPLUS

CN 9H-Purin-2-amine, 6-(phenylmethoxy)- (CA INDEX NAME)



REFERENCE COUNT: 159 THERE ARE 159 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 12 OF 41 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2002:81642 CAPLUS Full-text

DOCUMENT NUMBER: 137:72733

TITLE: An approach to the evaluation of the activity of the DNA repair enzyme O6-methylguanine-DNA-methyl-transferase in tumor tissue in vivo: syntheses of 6-benzyloxy-9-(2-[18F]fluoroethyl)-9H-purin-2-yl-amine and 6-benzyloxy-7-(2-[18F]fluoroethyl)-7H-purin-2-yl-amine

AUTHOR(S): Schirrmacher, Ralf; Nesseler, Esther; Hamkens, Wilhelm; Eichhorn, Uta; Schreckenberger, Mathias; Kaina, Bernd; Rosch, Frank

CORPORATE SOURCE: Institute of Nuclear Chemistry, Johannes Gutenberg-Universitat Mainz, Mainz, D-55128, Germany

SOURCE: Applied Radiation and Isotopes (2002), 56(3), 511-517
CODEN: ARISEF; ISSN: 0969-8043

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The resistance of tumor cells to the cytostatic activity of methylating and chloroethylating anticancer drugs is determined by the level of expression of the DNA repair protein O6-methylguanine-DNA-methyl-transferase (MGMT). The synthesis of labeled 6-benzyloxy-9H-purin-2-ylamine derivs. should hence allow a quantification of the MGMT status of tumor and non-target tissue in vivo. 6-Benzyloxy-9-(2-fluoroethyl)-9H-purin-2-yl-amine and 6-benzyloxy-7-(2-fluoroethyl)-7H-purin-2-yl-amine were synthesized and evaluated in vitro, both showing an affinity of 1.8 μM. 6-Benzyloxy-9-(2-[18F]fluoroethyl)-9H-purin-2-yl-amine and 6-benzyloxy-7-(2-[18F]fluoroethyl)-7H-purin-2-yl-amine were synthesized by alkylation of 6-benzyloxy-9H-purin-2-ylamine with 1-[18F]fluoro-2- tosylethane in optimized yields of 41% and 20%, resp. Biodistribution studies were performed in nude mice, carrying mex+ (MGMT expressing) and mex- tumors.

CC 1-6 (Pharmacology)
Section cross-reference(s): 14, 26, 28

IT ***19916-73-5P*** 334652-83-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(approach to evaluation of activity of DNA repair enzyme O6-methylguanine-DNA-Me-transferase in tumor tissue in vivo by syntheses of labeled 6-benzyloxy-9H-purin-2-ylamine derivs. in relation

to drug resistance)

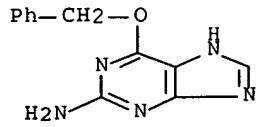
IT *19916-73-5P*

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(approach to evaluation of activity of DNA repair enzyme O6-methylguanine-DNA-Me-transferase in tumor tissue in vivo by syntheses of labeled 6-benzyloxy-9H-purin-2-ylamine derivs. in relation to drug resistance)

RN 19916-73-5 CAPLUS

CN 9H-Purin-2-amine, 6-(phenylmethoxy)- (CA INDEX NAME)



REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 13 OF 41 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2001:787185 CAPLUS Full-text

DOCUMENT NUMBER: 136:53967

TITLE: Monosaccharide-Linked Inhibitors of O6-Methylguanine-DNA Methyltransferase (MGMT): Synthesis, Molecular Modeling, and Structure-Activity Relationships

AUTHOR(S): Reinhard, Jost; Hull, William E.; von Lieth, Claus-Wilhelm; Eichhorn, Uta; Kliem, Hans-Christian; Kaina, Bernd; Wiessler, Manfred

CORPORATE SOURCE: Division of Molecular Toxicology and Central Spectroscopy Department, German Cancer Research Center, Heidelberg, D-69009, Germany

SOURCE: Journal of Medicinal Chemistry (2001), 44(24), 4050-4061

CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 136:53967

AB A series of potential inhibitors of the human DNA repair protein O6-methylguanine-DNA methyltransferase (MGMT) were synthesized, characterized in detail by NMR, and tested for their ability to deplete MGMT activity in vitro. The new compds., ω-[O6-R-guanin-9-yl]- (CH2)n-β-D-glucosides with R = benzyl or 4-bromothenyl and ω = n = 2, 4, ... 12, were compared with the established inhibitors O6-benzylguanine (O6-BG), 8-aza-O6-benzylguanine (8-aza-BG), and O6-(4-bromothenyl)guanine (4-BTG), which exhibit in an in vitro assay IC50 values of 0.62, 0.038, and 0.009 μM, resp. Potential advantages of the glucosides are improved water solubility and selective uptake in tumor cells. The 4-BTG glucosides with n = 2, 4, 6 show moderate inhibition with an IC50 of ca. 0.5 μM, while glucosides derived from BG and 8-aza-BG showed significantly poorer inhibition compared to the parent compds. The 4-BTG glucosides with n = 8, 10, 12 were effective inhibitors with IC50 values of ca. 0.03 μM. To understand this behavior, extensive mol. modeling studies were performed using the published crystal structure of MGMT (PDB entry: 1QNT). The inhibitor mols. were docked into the BG binding pocket, and mol. dynamics simulations

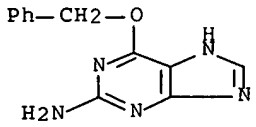
with explicit water mols. were carried out. Stabilization energies for the interactions of specific regions of the inhibitor and individual amino acid residues were calculated The alkyl spacer is located in a cleft along helix 6 of MGMT. With increasing spacer length there is increasing interaction with several amino acid residues which play an important role in the proposed nucleotide flipping mechanism required for DNA repair.

CC 33-7 (Carbohydrates)
Section cross-reference(s): 7, 34, 75

IT 6301-83-3P ***19916-73-5P*** 192441-08-0P 382607-70-7P
382607-72-9P 382607-74-1P 382607-76-3P 382607-78-5P 382607-80-9P
382607-81-0P 382607-83-2P 382607-85-4P
RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis mol. modeling and structure activity relationships of monosaccharide-linked inhibitors of O6-methylguanine-DNA methyltransferase)

IT ***19916-73-5P***
RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis mol. modeling and structure activity relationships of monosaccharide-linked inhibitors of O6-methylguanine-DNA methyltransferase)

RN 19916-73-5 CAPLUS
CN 9H-Purin-2-amine, 6-(phenylmethoxy)- (CA INDEX NAME)



REFERENCE COUNT: 48 THERE ARE 48 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 14 OF 41 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:333644 CAPLUS Full-text
DOCUMENT NUMBER: 134:353553
TITLE: Preparation of double-stranded peptide nucleic acids
INVENTOR(S): Norden, Benget; Wittung, Pernilla; Buchardt, Ole; Egholm, Michael; Nielsen, Peter E.; Berg, Rolf
PATENT ASSIGNEE(S): Swed.
SOURCE: U.S., 62 pp., Cont.-in-part of U.S. 5,539,082.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 19
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6228982	B1	20010508	US 1993-88661	19930702
WO 9220702	A1	19921126	WO 1992-EP1219	19920522
W: AT, AU, BB, BG, BR, CA, CH, CS, DE, DK, ES, FI, GB, HU, JP, KP, KR, LK, LU, MG, MN, MW, NL, NO, PL, RO, RU, SD, SE, US				
RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FR, GA, GB, GN, GR, IT, LU, MC, ML, MR, NL, SE, SN, TD, TG				
US 5539082	A	19960723	US 1993-54363	19930426

EP 1310507	A2	20030514	EP 2003-75412	19940425
EP 1310507	A3	20040317		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE				
CA 2166462	A1	19950112	CA 1994-2166462	19940701
WO 9501369	A1	19950112	WO 1994-IB211	19940701
W: CA, JP				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
EP 717750	A1	19960626	EP 1994-919803	19940701
EP 717750	B1	20021002		
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JP 09509435	T	19970922	JP 1994-503384	19940701
AT 225369	T	20021015	AT 1994-919803	19940701
US 5773571	A	19980630	US 1996-595387	19960201
US 6441130	B1	20020827	US 1998-765798	19980628
JP 11310593	A	19991109	JP 1998-341582	19981201
JP 3273135	B2	20020408		
US 6610650	B1	20030826	US 2000-610264	20000706
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US 2003232355	A1	20031218	US 2003-348246	20030121

PRIORITY APPLN. INFO.:	WO 1992-EP1219	A2	19920522
	US 1993-54363	A2	19930426
	DK 1991-986	A	19910524
	DK 1991-987	A	19910524
	DK 1992-510	A	19920415
	US 1993-88658	A2	19930702
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	US 1993-108591	A2	19931122
	EP 1994-915682	A3	19940425
	JP 1994-524084	A3	19940425
	WO 1994-IB211	W	19940701
	US 1994-275951	A2	19940715
	WO 1995-US9084	W	19950713
	US 1998-765798	A3	19980628
	US 2000-610624	A3	20000705

AB A novel class of compds., known as peptide nucleic acids, form double-stranded structures with one another and with ssDNA. The peptide nucleic acids generally comprise ligands such as naturally occurring DNA bases attached to a peptide backbone through a suitable linker. Claimed is a composition comprising two polymeric strands which are hydrogen bonded to each other. Each strand has the formula Q-C1-B1(A1-L1)-D1-G1-C2-B2(A2-L2)- D2-G2-Cn-Bn(An-Ln)-Dn-I [n is at least 2; each L1-Ln is independently selected from H, OH, (C1-C4)alkanoyl, (non)naturally occurring nucleobases, aromatic moieties, DNA intercalators, nucleobase-binding groups, heterocyclic moieties, and reporter ligands; each C1-Cn and each D1-Dn is identical and has the formula (CR6R7)y and (CR6R7)z, resp., where each y and z is 0-10, the sum y + z being greater than 2 but not more than 10 and R6 is H and R7 is the side chain of a naturally occurring α-amino acid or R6 and R7 are H, alkyl, aryl, aralkyl, hydroxy, etc.; each G1-Gn-1 is identical and has the formula NR3CO, NR3CS, NR3SO or NR3SO2; each A1-An and each B1-Bn is identical, where A is (CR1R2)p-Y-(CR1R2)q (Z), Z-C(X) or Z-NR3CO (p, q = 0-5; Y is a single bond, O, S or NR4; X = O, S, Se, NR3, CH2, CMe2; R1-R4 = H, alkyl, alkoxy, hydroxy, amino, etc.) and B is N or R3N+ or A is Z-C(:X)NR3 and B is CH; Q is CO2H, CONR'R'', SO3H, SONR'R'' or an activated derivative of CO2H or SO3H; I is NHR'''R'''' or NR'''C(O)R'''' (R', R'', R''' and R'''' are selected from H, alkyl, an amino protecting groups, reporter ligands, intercalators, chelators, peptides, proteins, carbohydrates, lipids, steroids, nucleosides, nucleotides, nucleotide diphosphates, nucleotide triphosphates, oligonucleotides, oligonucleosides and soluble and non-soluble polymers)]. Thus, preparation, binding and helix formation of complementary antiparallel PNA strands H-GTAGATCACT-LysNH2 and H-AGTGATCTAC-LysNH2 was studied. The CD spectra of the

PNA 10-mers are almost vanishingly small, indicating that there is no preferred helical stacking of bases. However, a strong CD spectrum arises upon titration of one 10-mer with the complementary 10-mer, a saturation obtained at about 1:1 stoichiometry. The CD spectrum resembles that of β-DNA, indicating a right-handed helix. It is believed that a PNA-PNA complex having no preferred helicity initially is formed. The kinetics by which this double-stranded structure reorganizes into a uniform, right-handed double helix has been monitored and the activation parameters for the process determined

IC ICM C07K005-00
ICS C12Q001-68

INCL 530300000

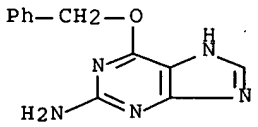
CC 34-3 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 6, 33

IT 4113-97-7P 5236-60-2P 6214-59-1P 13303-10-1P ***19916-73-5P***
20924-05-4P 25477-96-7P 31385-63-4P 34046-07-6P 57260-73-8P
72648-80-7P 72648-81-8P 89459-22-3P 89711-08-0P 90495-99-1P
128421-86-3P 137618-48-5P 139166-79-3P 139166-80-6P 139166-81-7P
139166-82-8P 139924-84-8P 142611-64-1P 144564-94-3P 144564-95-4P
148273-98-7P 149035-00-7P 149035-01-8P 149035-02-9P 149035-03-0P
149376-49-8P 149376-50-1P 149376-51-2P 149376-53-4P 149376-58-9P
149376-66-9P 149376-67-0P 149376-68-1P 149376-69-2P 149376-70-5P
149376-72-7P 149376-73-8P 149376-76-1P 149376-78-3P 149376-79-4P
149376-80-7P 149376-81-8P 149376-82-9P 149376-83-0P 149376-97-6P
149376-98-7P 149376-99-8P 149411-91-6P 149411-92-7P 149411-93-8P
149411-94-9P 149465-96-3P 149465-97-4P 149465-98-5P 149465-99-6P
158097-21-3P 176026-20-3P 202999-51-7P 202999-52-8P 203134-16-1P
203134-20-7P 203265-72-9P 339034-88-7P 339034-89-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of double-stranded peptide nucleic acids)

IT ***19916-73-5P***
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of double-stranded peptide nucleic acids)

RN 19916-73-5 CAPLUS

CN 9H-Purin-2-amine, 6-(phenylmethoxy)- (CA INDEX NAME)



REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 15 OF 41 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:91538 CAPLUS Full-text
DOCUMENT NUMBER: 134:147852
TITLE: Synthesis of acyclic nucleoside derivatives
INVENTOR(S): Leanna, M. Robert; Hannick, Steven M.; Rasmussen, Michael; Tien, Jien-Heh J.; Bhagavatula, Lakshmi; Singam, Pulla Reddy; Gates, Bradley D.; Kolaczkowski, Lawrence; Patel, Ramesh R.; Wayne, Greg; Lannoye, Greg; Zhang, Weijiang; Tian, Zhenping; Lukin, Kirill A.; Narayanan, Bikshandarkoil A.; Riley, David A.;

Morton, Howard; Chang, Sou-Jen; Curty, Cynthia B.; Plata, Daniel; Bellettini, John; Shelat, Bhadra; Spitz, Tiffany; Yang, Cheng-Xi

PATENT ASSIGNEE(S): Mediver AB, Swed.

SOURCE: U.S., 41 pp., Cont.-in-part of U.S. Ser. No. 20,231, abandoned.
CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 5

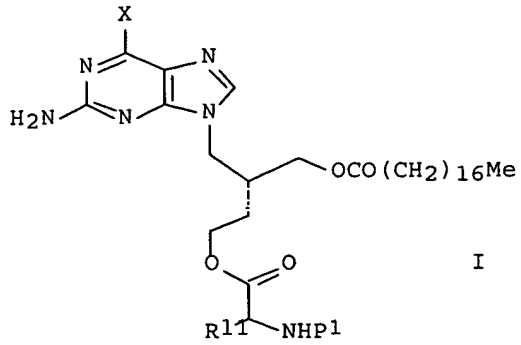
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6184376	B1	20010206	US 1998-130214	19980806
CA 2339250	A1	20000217	CA 1999-2339250	19990805
WO 2000008025	A1	20000217	WO 1999-SE1339	19990805
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 9961271	A	20000228	AU 1999-61271	19990805
AU 765286	B2	20030911		
EP 1131323	A1	20010912	EP 1999-948005	19990805
EP 1131323	B1	20050427		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
JP 2002522439	T	20020723	JP 2000-563658	19990805
AT 294179	T	20050515	AT 1999-948005	19990805
EP 1535923	A1	20050601	EP 2005-1026	19990805
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY				
ES 2237942	T3	20050801	ES 1999-948005	19990805
US 6613936	B1	20030902	US 2000-692599	20001018
IN 2001MN00121	A	20050304	IN 2001-MN121	20010202
US 2004024214	A1	20040205	US 2002-315580	20021209
US 6878844	B2	20050412		
US 2004248910	A1	20041209	US 2004-871751	20040617
US 2005250795	A1	20051110	US 2005-131646	20050518

PRIORITY APPLN. INFO.:		
US 1997-37517P	P	19970210
US 1997-55153P	P	19970808
US 1998-20231	B2	19980206
US 1998-130214	A	19980806
EP 1999-948005	A3	19990805
WO 1999-SE1339	W	19990805
US 2000-692599	A3	20001018
US 2002-315580	A3	20021209
US 2004-871751	A3	20040617

OTHER SOURCE(S): MARPAT 134:147852

GI



I

AB Acyclic nucleoside derivs., including amino acid derivs. I (X = Br or iodo; R11 = iso-Pr or isobutyl; P1 is an N-protecting group), were prepared for use as pharmaceuticals. Thus, (R)-9-[2-(stearoyloxymethyl)-4-(L-valyloxy)butyl]guanine monohydrochloride was prepared from 9-[4-hydroxy-2-(hydroxymethyl)butyl]guanine (H2G) and shown to have antiviral activity significantly greater than that of acyclovir.

IC ICM C07D473-18
ICS C07D473-40; C07D317-30; C07F007-18; C12P017-18

INCL 544229000

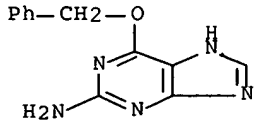
CC 34-2 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 10, 33, 63

IT 10084-80-7P ***19916-73-5P*** 195157-23-4P 195157-26-7P
211374-30-0P 211374-33-3P 211374-38-8P 256949-13-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(synthesis of acyclic nucleoside derivs.)

IT ***19916-73-5P***
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(synthesis of acyclic nucleoside derivs.)

RN 19916-73-5 CAPLUS

CN 9H-Purin-2-amine, 6-(phenylmethoxy)- (CA INDEX NAME)



REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 16 OF 41 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2000:119594 CAPLUS Full-text
DOCUMENT NUMBER: 132:279045
TITLE: Synthesis of 6-aryloxy- and 6-arylalkoxy-2-

chloropurines and their interactions with purine nucleoside phosphorylase from Escherichia coli

AUTHOR(S): Bzowska, Agnieszka; Magnowska, Lucyna; Kazimierczuk, Zygmunt

CORPORATE SOURCE: Department of Biophysics, Institute of Experimental Physics, University of Warsaw, Warsaw, 02 089, Pol.

SOURCE: Zeitschrift fuer Naturforschung, C: Journal of Biosciences (1999), 54(12), 1055-1067
CODEN: ZNCBDA; ISSN: 0939-5075

PUBLISHER: Verlag der Zeitschrift fuer Naturforschung

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The phase transfer method was applied to perform the nucleophilic substitution of 2,6-dichloropurines by modified arylalkyl alc. or phenols. Since under these conditions only the 6-halogen is exchanged, this method gives 2-chloro-6-aryloxy- and 2-chloro-6-arylalkoxy-purines. 2-Chloro-6-benzylthiopurine was synthesized by alkylation of 2-chloro-6-thiopurine with benzyl bromide. The stereoisomers of 2-chloro-6-(1-phenyl-1-ethoxy)purine were obtained from R- and S-enantiomers of sec.-phenylethyl alc. and 2,6-dichloropurine. All derivs. were tested for inhibition with purified hexameric E. coli purine nucleoside phosphorylase (PNP). For analogs showing IC50 < 10 μM, the type of inhibition and inhibition consts. were determined In all cases the exptl. data were best described by the mixed-type inhibition model and the uncompetitive inhibition constant, Kiu, was found to be several-fold lower than the competitive inhibition constant, Kic. This effect seems to be due to the 6-aryloxy- or 6-arylalkoxy substituent, because a natural PNP substrate adenine, as well as 2-chloroadenine, show mixed type inhibition with almost the same inhibition consts. Kiu and Kic. The most potent inhibition was observed for 6-benzylthio-2-chloro-, 6-benzyloxy-2-chloro-, 2-chloro-6-(2-phenyl-1-ethoxy), 2-chloro-6-(3-phenyl-1-propoxy)- and 2-chloro-6-ethoxypurines (Kiu = 0.4, 0.6, 1.4, 1.4 and 2.2 μM, resp.). The R-stereoisomer of 2-chloro-6-(1-phenyl-1-ethoxy)purine has Kiu = 2.0 μM, whereas inhibition of its S counterpart is rather weak (IC50 > 12 μM). More rigid (e.g. phenoxy-), non-planar (cyclohexyloxy-), or more bulky (2,4,6-trimethylphenoxy-) substituents at position 6 of the purine base gave less potent inhibitors (IC50 = 26, 56 and >100 μM, resp.). The derivs. are selective inhibitors of hexameric "high-mol. mass" PNPs because no inhibitory activity vs. trimeric Cellulomonas sp. PNP was detected. By establishing the ligand-dependent stabilization pattern of the E. coli PNP it was shown that the new derivs., similarly as the natural purine bases, are able to form a dead-end ternary complex with the enzyme and orthophosphate. It was also shown that the derivs. are substrates in the reverse synthetic direction catalyzed by E. coli PNP.

CC 26-9 (Biomolecules and Their Synthetic Analogs)
Section cross-reference(s): 1, 9

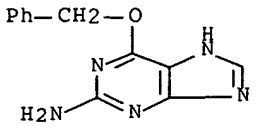
IT 1198-46-5P ***19916-73-5P*** 20366-94-3P 104121-30-4P
237422-18-3P 237422-19-4P 237422-20-7P 237422-21-8P 237422-22-9P
237422-23-0P 263715-65-7P 263715-66-8P 263715-67-9P 263715-68-0P
263715-69-1P 263715-70-4P 263715-71-5P 263715-72-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis of 6-aryloxy- and 6-arylalkoxy-2-chloropurines and their interactions with purine nucleoside phosphorylase from Escherichia coli)

IT ***19916-73-5P***
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(synthesis of 6-aryloxy- and 6-arylalkoxy-2-chloropurines and their interactions with purine nucleoside phosphorylase from Escherichia coli)

RN 19916-73-5 CAPLUS

CN 9H-Purin-2-amine, 6-(phenylmethoxy)- (CA INDEX NAME)



REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 17 OF 41 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1999:745349 CAPLUS Full-text

DOCUMENT NUMBER: 132:93577

TITLE: Synthesis of C-5'-nor-dideoxycarbanucleosides structurally related to neplanocin C

AUTHOR(S): Comin, Maria J.; Pujol, Carlos A.; Damonte, Elsa B.; Rodriguez, Juan B.

CORPORATE SOURCE: Departamento de Quimica Organica, and Facultad de Ciencias Exactas y Naturales, Universidad de Buenos Aires, Buenos Aires, RA-1428, Argent.

SOURCE: Nucleosides & Nucleotides (1999), 18(10), 2219-2231
CODEN: NUNUD5; ISSN: 0732-8311

PUBLISHER: Marcel Dekker, Inc.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Purine carbanucleosides built on a 6-oxabicyclo[3.1.0]hexane template were synthesized from readily available 2-cyclopentenone employing a Mitsunobu reaction to incorporate the base onto the carbocyclic ring. Both adenosine and guanosine analogs exhibited moderate antiviral activity.

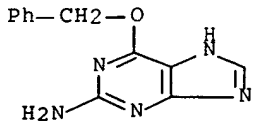
CC 33-9 (Carbohydrates)

IT 3212-60-0P, 2-Cyclopenten-1-ol ***19916-73-5P*** 29782-88-5P 254751-97-8P 254751-98-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis of C-nor-dideoxycarbanucleosides structurally related to neplanocin C)

IT ***19916-73-5P***
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis of C-nor-dideoxycarbanucleosides structurally related to neplanocin C)

RN 19916-73-5 CAPLUS

CN 9H-Purin-2-amine, 6-(phenylmethoxy)- (CA INDEX NAME)

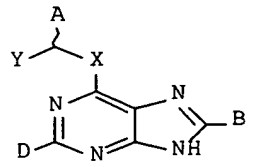


REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

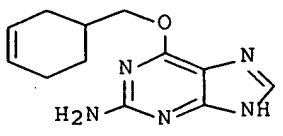
L18 ANSWER 18 OF 41 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1999:64689 CAPLUS Full-text
DOCUMENT NUMBER: 130:139576
TITLE: Preparation of cyclin dependent kinase inhibiting purine derivatives
INVENTOR(S): Griffin, Roger John; Calvert, Alan Hilary; Curtin, Nicola Jane; Newell, David Richard; Golding, Bernhard Thomas; Endicott, Jane Anne; Noble, Martin Edward Mantyla; Boyle, Francis Thomas; Jewsbury, Philip John
PATENT ASSIGNEE(S): Newcastle University Ventures Limited, UK
SOURCE: PCT Int. Appl., 92 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 9902162	A1	19990121	WO 1998-GB2025		19980710
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW					
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG					
CA 2294244	A1	19990121	CA 1998-2294244		19980710
AU 9882342	A	19990208	AU 1998-82342		19980710
AU 744986	B2	20020307			
EP 1017394	A1	20000712	EP 1998-932413		19980710
EP 1017394	B1	20051207			
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY					
JP 2001509483	T	20010724	JP 2000-501753		19980710
AT 311884	T	20051215	AT 1998-932413		19980710
ES 2253821	T3	20060601	ES 1998-932413		19980710
US 6303618	B1	20011016	US 2000-481708		20000112
PRIORITY APPLN. INFO.:			GB 1997-14603	A	19970712
			GB 1998-6743	A	19980328
			WO 1998-GB2025	W	19980710

OTHER SOURCE(S): MARPAT 130:139576
GI



I



II

AB Purine derivs. I [X = O, S or CHRx; Rx = H, C1-4-alkyl; D = H, halo, NZ1Z2; Z1, Z2 = H, C1-4-alkyl, C1-4-hydroxyalkyl; A = H, C1-4-alkyl, C1-4-alkoxy, OH, CH2(CH2)nOH, NRa1Ra2; n = 1 - 4; Ra1, Ra2 = H, C1-4-alkyl; B = H, C1-4-alkyl, C1-4-alkoxy, CF3, (un)substituted aryl, (e.g. Ph), (un)substituted aralkyl (e.g. benzyl), hydroxy group that provides a C=O tautomer; Y = (un)substituted C4-8-carbocyclic, -heterocyclic ring, (un)substituted linear or branched hydrocarbon chain] which can act as inhibitors of cyclin dependent kinases (CDKs) and which thereby can provide useful therapeutic compds. for use in treatment of tumors or other cell proliferation disorders are disclosed. The compds. of this invention bind to CDK mols. in a manner that appears to be different to that of known CDK inhibitors such as olomoucine and roscovitine. Thus, O6-[(cyclohex-3-en-1-yl)methyl]guanine (II) was prepared from 2-amino-6-chloropurine via addition to 3-cyclohexenemethanol in THF containing sodium hydride. II is an active inhibitor of cyclin dependent kinases: IC50 = 3.2 μM vs. CDK1, 87% inhibition of CDK2 at 100μM and 53% inhibition of CDK4.

IC ICM A61K031-52
ICS A61K031-70; C07D473-18; C07D473-24; C07D473-26; C07D473-40; C07H017-02

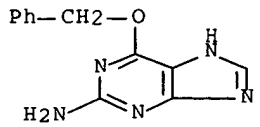
CC 33-3 (Carbohydrates)
Section cross-reference(s): 1, 26

IT 1005-37-4P, 2-Amino-4-chloro-6-(methylamino)pyrimidine 6331-91-5P, O6-Propylguanine ***19916-73-5P***, O6-Benzylguanine 20535-83-5P 50663-54-2P, O6-Allylguanine 51866-19-4P 57500-07-9P, 6-(Benzyloxy)purine 76412-62-9P 100061-59-4P, 2,6-Diamino-4-(benzyloxy)pyrimidine 101622-51-9DP, Olomoucine, analogs 101724-61-2P, 2,6-Diamino-4-(benzyloxy)-5-nitrosopyrimidine 105217-88-7P, 6-(2-Phenylethoxy)purine 146331-47-7P, 6-(Allyloxy)purine 158754-46-2P, NU 6043 161058-73-7P, O6-Acetonylguanine 161058-75-9P, 2-Amino-6-(3-methyl-2-oxobutyloxy)purine 161058-76-0P, 2-Amino-6-(2-oxo-2-phenylethoxy)purine 161058-77-1P, O6-(Methally)guanine 161058-78-2P, O6-(Ethallyl)guanine 161058-79-3P, O6-(Isopropallyl)guanine 161058-80-6P, O6-(2-Phenylallyl)guanine 161058-81-7P, 2-Amino-N7-allyl-6-allyloxypurine 161058-82-8P, 2-Amino-6-(3-methylbutyloxy)purine 161058-83-9P, O6-(Cyclohexylmethyl)guanine 161058-84-0P, O6-(Phenethoxy)guanine 161058-86-2P, 2-Amino-6-(2,2-dimethoxybutyloxy)purine 161058-88-4P, 2-Amino-6-(2,2-dimethoxy-2-phenylethyloxy)purine 162320-36-7P, 2-Amino-6-[(2-furanyl)methoxy]purine 162320-40-3P, 2-Amino-6-(3-pyridylmethoxy)purine 162320-42-5P, 2-Amino-6-(2-naphthylmethyloxy)purine 162320-51-6P, 2-Amino-6-(1-naphthylmethyloxy)purine 186692-46-6DP, Roscovitine, analogs 188680-41-3P, O6-Propargylguanine 188680-42-4P, O6-(Cyclopentylmethyl)guanine 188680-43-5P, O6-(1-Cyclopentenylmethyl)guanine 219991-55-6P, O6-(D-Ribofuranos-5-yl)guanine 219991-56-7P, O6-(1,4-Dioxan-2-ylmethyl)guanine 219991-57-8P 219991-58-9P, 2-Amino-6-(cyclohexylmethylthio)purine 219991-59-0P 219991-60-3P 219991-61-4P 219991-62-5P, 2-Amino-6-[(uracil-5-

yl)methoxy]-8-oxopurine 219991-63-6P, 2-Amino-6-[(uracil-5-yl)methylthio]-8-oxopurine 219991-64-7P, 2-Amino-6-[cyclohexenylmethoxy]-8-oxopurine 219991-65-8P, 2-Amino-6-[cyclohexenylmethylthio]-8-oxopurine 219991-66-9P, O6-(D-Galactos-6-yl)guanine 220028-00-2P, 6-(2-Tetrahydropyranylmethoxy)purine 220028-09-1P, 6-(Cyclohexylmethoxy)purine 220033-58-9P, NU 2077 220034-21-9P, NU 6022 220035-58-5P, 2-Amino-N9-allyl-6-(allyloxy)purine 220035-63-2P, 2-Amino-6-(allyloxy)-N9-benzylpurine 220035-67-6P, 2-Amino-6-(2,3-dihydroxypropoxy)purine 220035-74-5P, 2-Amino-6-(2,3-dimethoxypropoxy)purine 220035-77-8P, 2-(N,N-Dimethylamino)-6-(allyloxy)purine 220035-88-1P, 2-Amino-6-(5-hexenyloxy)purine 220035-91-6P, O6-Heptylguanine 220035-93-8P, 2-Amino-6-[(E)-hex-3-enyloxy]purine 220035-95-0P, 2-Amino-6-[(cyclohex-3-enylmethyl)oxy]purine 220035-96-1P, O6-(1-Cyclohexenylmethyl)guanine 220035-97-2P, NU 6012 220035-98-3P, 2-Amino-6-(2-tetrahydrofuranylmethyloxy)purine 220035-99-4P, 2-Amino-6-[(1-adamantylmethyl)oxy]purine 220036-00-0P, NU 6017 220036-01-1P, 2-Amino-6-(2-tetrahydropyranylmethyloxy)purine 220036-02-2P, 2-Amino-6-(2,3-dihydroxypropoxy)purine acetonide 220036-04-4P, 2-Amino-6-(2-cyclohexylethyloxy)purine 220036-05-5P, NU 6024 220036-06-6P, NU 6025 220036-07-7P, O6-(1,4-Benzodioxan-2-ylmethyl)guanine 220036-08-8P, 2,6-Diamino-4-(cyclohexylmethoxy)-5-nitrosopyrimidine 220036-09-9P, 2-Amino-6-(1-cyclohexylethoxy)purine 220036-10-2P, NU 6030 220036-11-3P, NU 6031 220036-12-4P, NU 6032 220036-13-5P, 2-Amino-6-(cyclohexylmethoxy)-8-oxopurine 220036-14-6P, 2,6-Diamino-4-(cyclohexylmethoxy)pyrimidine 220036-16-8P, NU 6037 220036-18-0P, NU 6041 220036-19-1P, NU 6044 220036-20-4P, 2,6-Diamino-4-(3-cyclohexenylmethoxy)-5-nitrosopyrimidine 220036-21-5P, 2,6-Diamino-4-(3-cyclohexenylmethoxy)pyrimidine 220036-23-7P, 2-(Dimethylamino)-6-(cyclohexylmethoxy)purine
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of purine derivs. as cyclin dependent kinase inhibitors)

IT ***19916-73-5P***, O6-Benzylguanine
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of purine derivs. as cyclin dependent kinase inhibitors)

RN 19916-73-5 CAPLUS
CN 9H-Purin-2-amine, 6-(phenylmethoxy)- (CA INDEX NAME)



REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 19 OF 41 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1998:550409 CAPLUS Full-text
DOCUMENT NUMBER: 129:175918
TITLE: Synthesis and bioavailability of acyclic nucleosides as antiviral agents
INVENTOR(S): Leanna, M. Robert; Hannick, Steven M.; Rasmussen,

Michael; Tien, Jien-Heh J.; Bhagavatula, Lakshmi; Singam, Pulla Reddy; Gates, Bradley D.; Kolaczkowski, Lawrence; Patel, Ramesh R.; Wayne, Greg; Lannoye, Greg; Zhang, Weijiang; Tian, Zhenping; Lukin, Kirill L.; Narayanan, Bikshandarkor A.; Riley, David A.; Morton, Howard; Chang, Sou-jen

PATENT ASSIGNEE(S): Abbott Laboratories, USA

SOURCE: PCT Int. Appl., 109 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 5

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9834917	A2	19980813	WO 1998-US2439	19980206
WO 9834917	A3	19990114		
W: CA, JP, MX				
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
US 5869493	A	19990209	US 1997-798216	19970210
CA 2277151	A1	19980813	CA 1998-2277151	19980206
EP 971923	A2	20000119	EP 1998-906239	19980206
EP 971923	B1	20021106		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI				
JP 2001512442	T	20010821	JP 1998-534963	19980206
AT 227289	T	20021115	AT 1998-906239	19980206
ES 2186127	T3	20030501	ES 1998-906239	19980206
US 6255312	B1	20010703	US 1998-146194	19980903
ES 2237942	T3	20050801	ES 1999-948005	19990805
MX 9907340	A	20000531	MX 1999-7340	19990809
US 6576763	B1	20030610	US 2000-550554	20000417
US 2002188125	A1	20021212	US 2002-76833	20020214
US 6703394	B2	20040309		
US 2004132749	A1	20040708	US 2003-741615	20031219

PRIORITY APPLN. INFO.:		
US 1997-37517P	P	19970210
US 1997-798216	A	19970210
US 1997-908754	A	19970808
SE 1996-613	A	19960216
SE 1996-614	A	19960216
WO 1998-US2439	W	19980206
US 1998-146194	A3	19980903
EP 1999-948005	A	19990805
US 2000-550554	A3	20000417
US 2002-76833	A3	20020214

OTHER SOURCE(S): MARPAT 129:175918

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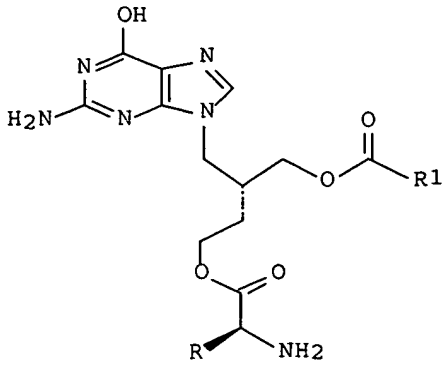


I

AB Acyclic nucleosides I (R = iPr, iBu; R1 = C3-C21 saturated or mono-unsatd. alkyl) were prepared as virucides. Thus, (R)-9-[2-(stearoyloxymethyl)-4-(L-valyloxy)butyl]guanine was prepared and tested for its bioavailability (56%) in rats and monkeys and for its HSV-1 activity in mice.

IC ICM C07D073-00

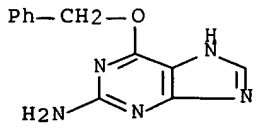
CC 33-9 (Carbohydrates)
Section cross-reference(s): 1, 34, 63

IT 10084-80-7P, N-(Benzyloxycarbonyl)valine anhydride ***19916-73-5P***, 2-Amino-6-Benzyloxypurine 21339-47-9P 55387-85-4P 195157-13-2P 195157-14-3P 195157-15-4P 195157-16-5P 195157-17-6P 195157-18-7P 195157-19-8P 195157-20-1P 195157-21-2P 195157-22-3P 195157-23-4P 195157-25-6P 195157-26-7P 195157-27-8P 195157-28-9P 195157-29-0P 195157-30-3P 195157-35-8P 195157-37-0P 195157-38-1P 211374-30-0P 211374-32-2P 211374-33-3P 211374-34-4P 211374-36-6P 211374-37-7P 211374-38-8P 211374-39-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis and bioavailability of acyclic nucleosides as antiviral agents)

IT ***19916-73-5P***, 2-Amino-6-Benzyloxypurine
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis and bioavailability of acyclic nucleosides as antiviral agents)

RN 19916-73-5 CAPLUS

CN 9H-Purin-2-amine, 6-(phenylmethoxy)- (CA INDEX NAME)

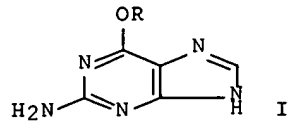


L18 ANSWER 20 OF 41 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1998:535782 CAPLUS Full-text
DOCUMENT NUMBER: 129:216464
TITLE: Preparation of 2-aminopurine derivatives
INVENTOR(S): Uefuji, Tamio; Watanabe, Yosuke

PATENT ASSIGNEE(S): Sumika Fine Chemicals Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 4 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 10218880	A	19980818	JP 1997-44576	19970212

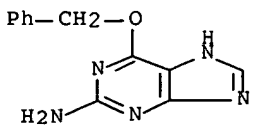
PRIORITY APPLN. INFO.: JP 1997-44576 19970212
OTHER SOURCE(S): CASREACT 129:216464; MARPAT 129:216464
GI



I

AB The derivs. I [R = (un)substituted C6-12 aryl, (un)substituted C7-13 aralkyl], useful as intermediates for nucleoside antiviral agents, are prepared by treatment of NaOH or KOH with ROH in organic solvents capable of azeotropically removing H2O, and treatment of the resulting ROK or RONa with 2-amino-6-chloropurine (II). I prepared as described above may be extracted with aqueous alkali solns. and crystallized with acids. A mixture of NaOH, PhCH2OH, and toluene was heated at 130° to while removing H2O and toluene. The resulting PhCH2ONa was treated with II at 70° for 5 h, and the reaction mixture was mixed with toluene and extracted with an aqueous NaOH solution The aqueous layer was washed with toluene and acidified with an aqueous HCl to give 97.0% I (R = CH2Ph).

IC ICM C07D473-18
CC 26-9 (Biomolecules and Their Synthetic Analogs)
IT ***19916-73-5P***, 2-Amino-6-benzyloxypurine
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(preparation of amino(aryloxy or aralkyloxy)purines by treatment of aminochloropurine with alkoxides formed from NaOH or KOH and alcs.)
IT ***19916-73-5P***, 2-Amino-6-benzyloxypurine
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(preparation of amino(aryloxy or aralkyloxy)purines by treatment of aminochloropurine with alkoxides formed from NaOH or KOH and alcs.)
RN 19916-73-5 CAPLUS
CN 9H-Purin-2-amine, 6-(phenylmethoxy)- (CA INDEX NAME)



L18 ANSWER 21 OF 41 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1998:441926 CAPLUS Full-text
DOCUMENT NUMBER: 129:122864
TITLE: Preparation of peptide nucleic acids having enhanced binding affinity and sequence specificity
INVENTOR(S): Burchardt, Ole; Egholm, Michael; Nielsen, Peter Eigil; Berg, Rolf Henrik; Burchardt, Dorte
PATENT ASSIGNEE(S): Isis Pharmaceuticals, Inc., Den.
SOURCE: U.S., 72 pp., Cont.-in-part of U. S. Ser. No. 108,591.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 19
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5766855	A	19980616	US 1996-686113	19960724
CA 2109320	A1	19921125	CA 1992-2109320	19920522
CA 2109320	C	20030722		
AU 9218806	A	19921230	AU 1992-18806	19920522
AU 666480	B2	19960215		
EP 586618	A1	19940316	EP 1992-923579	19920522
EP 586618	B1	19970716		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
JP 06509063	T	19941013	JP 1992-510139	19920522
EP 1074559	A1	20010207	EP 2000-203148	19920522
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC				
EP 1162206	A2	20011212	EP 2001-203303	19920522
EP 1162206	A3	20040414		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC				
JP 2003235590	A	20030826	JP 2003-15384	19920522
EP 1411063	A1	20040421	EP 2003-77836	19920522
EP 1411063	B1	20060719		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC				
US 6395474	B1	20020528	US 1993-108591	19931122
NO 9304235	A	19940120	NO 1993-4235	19931123
NO 313201	B1	20020826		
US 6357163	B1	20020319	US 1994-150156	19940504
US 5773571	A	19980630	US 1996-595387	19960201
CA 2261566	A1	19980129	CA 1997-2261566	19970724
WO 9803542	A1	19980129	WO 1997-US12811	19970724
W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AN				
RW: GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9738081	A	19980210	AU 1997-38081	19970724
AU 717387	B2	20000323		
EP 960121	A1	19991201	EP 1997-935053	19970724
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
JP 2000503671	T	20000328	JP 1998-507186	19970724
JP 3306073	B2	20020724		
JP 2002105059	A	20020410	JP 2001-222248	19970724

AT 311402	T	20051215	AT 1997-935053		19970724
US 6710164	B1	20040323	US 1999-230088		19990310
US 2002160383	A1	20021031	US 2001-983210		20011023
US 2003180734	A1	20030925	US 2002-154890		20020523
US 2006160731	A1	20060720	US 2003-691012		20031022
US 2006046255	A1	20060302	US 2005-29005		20050105
PRIORITY APPLN. INFO.:			DK 1991-986	A	19910524
			DK 1991-987	A	19910524
			DK 1992-510	A	19920415
			US 1993-108591	A2	19931122
			EP 1992-911165	A3	19920522
			EP 2000-203148	A3	19920522
			JP 1992-510139	A3	19920522
			WO 1992-EP1219	W	19920522
			WO 1992-EP1220	A	19920522
			US 1993-54363	A3	19930426
			US 1994-150156	A1	19940504
			US 1996-685484	A	19960724
			US 1996-686113	A	19960724
			US 1996-686114	A	19960724
			US 1996-686116	A	19960724
			US 1997-51002P	P	19970529
			JP 1998-507186	A3	19970724
			WO 1997-US12811	W	19970724
			US 2001-983210	B1	20011023
			US 2002-154890	A3	20020523

OTHER SOURCE(S): MARPAT 129:122864

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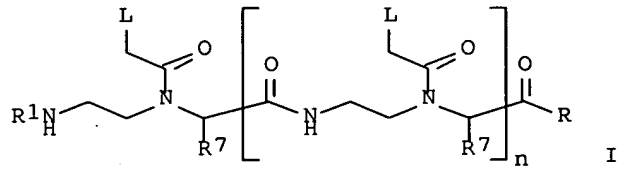


I

AB A novel peptide nucleic acids I [each L = naturally occurring and non-naturally occurring nucleobase, with the proviso that at least one L = 2,6-diaminopurine; each R7 = H, C1-8 alkylamine; R = OH, NH2, NH-Lys-NH2; R1 = H, Ac, Me3CO2C (Boc); n = 1-30] bind complementary DNA and RNA strands more strongly than a corresponding DNA strand, and exhibit increased sequence specificity and binding affinity. Methods of increasing binding affinity and sequence specificity of peptide nucleic acids are provided wherein some peptide nucleic acids comprise ligands selected from a group consisting of naturally-occurring nucleobases and non-naturally-occurring nucleobases attached to a polyamide backbone, while other peptide nucleic acids contain at least one 2,6-diaminopurine nucleobase and at least one C1 -C8 alkylamine side chain. A variety of peptide nucleic acid containing 2,6-diaminopurine and alkylamine side chains were prepared and exhibited enhanced sequence selectivity and binding affinities with complementary DNA and RNA strands.

IC ICM C12Q001-68

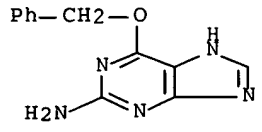
INCL 435006000

CC 34-3 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 1, 33

IT 4113-97-7P 5236-60-2P 6214-59-1P 13303-10-1P, tert-Butyl p-nitrophenyl carbonate ***19916-73-5P*** 20924-05-4P, 1-(Carboxymethyl)thymine 25477-96-7P 31385-63-4P 34046-07-6P 57260-73-8P 72648-80-7P 85301-38-8P 85301-50-4P 89459-22-3P 90495-99-1P 128421-86-3P 137618-48-5P 139166-79-3P 139166-80-6P 139166-81-7P 139166-82-8P 139924-84-8P 144564-94-3P 144564-95-4P 149035-00-7P 149035-01-8P 149035-02-9P 149035-03-0P 149376-49-8P 149376-50-1P 149376-51-2P 149376-66-9P 149376-67-0P 149376-68-1P 149376-69-2P 149376-70-5P 149376-71-6P 149376-72-7P 149376-73-8P 149376-74-9P 149376-76-1P 149376-78-3P 149376-79-4P 149376-80-7P 149376-81-8P 149376-82-9P 149376-83-0P 149411-91-6P 149411-92-7P 149411-93-8P 149411-94-9P 149465-96-3P 149465-97-4P 149465-98-5P 149494-90-6P 149500-73-2P 149500-74-3P 163081-00-3P 163081-01-4P 163081-06-9P 202343-70-2P 202343-71-3P 202999-28-8P 202999-51-7P 202999-52-8P 209331-73-7P 209331-76-0P 209331-79-3P 209331-82-8P 209332-02-5P 209332-04-7P 209332-06-9P 209332-10-5P 209332-12-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of peptide nucleic acids having enhanced binding affinity and sequence specificity)

IT ***19916-73-5P***
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of peptide nucleic acids having enhanced binding affinity and sequence specificity)

RN 19916-73-5 CAPLUS
CN 9H-Purin-2-amine, 6-(phenylmethoxy)- (CA INDEX NAME)



REFERENCE COUNT: 157 THERE ARE 157 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 22 OF 41 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1998:241026 CAPLUS Full-text
Correction of: 1998:115390
DOCUMENT NUMBER: 128:244346
Correction of: 128:177410
TITLE: Preparation of peptide nucleic acids having enhanced binding affinity, sequence specificity and solubility
INVENTOR(S): Buchardt, Ole; Egholm, Michael; Nielsen, Peter Eigil; Berg, Rolf Henrik
PATENT ASSIGNEE(S): Den.
SOURCE: U.S., 68 pp., Cont.-in-part of U.S. Ser. No. 108,591.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 19
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

US 5714331		A	19980203	US 1996-686116		19960724
CA 2109320		A1	19921125	CA 1992-2109320		19920522
CA 2109320		C	20030722			
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AU 666480		B2	19960215			
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US 5736336		A	19980407	US 1997-847108		19970501
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AU 717387		B2	20000323			
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AT 311402		T	20051215	AT 1997-935053		19970724
US 6710164		B1	20040323	US 1999-230088		19990310
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				EP 1992-911165	A3	19920522
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				WO 1992-EP1220	A	19920522
				US 1993-54363	A3	19930426
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US 1996-686113	A	19960724
US 1996-686114	A	19960724
US 1996-686116	A3	19960724
US 1997-51002P	P	19970529
JP 1998-507186	A3	19970724
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OTHER SOURCE(S): MARPAT 128:244346

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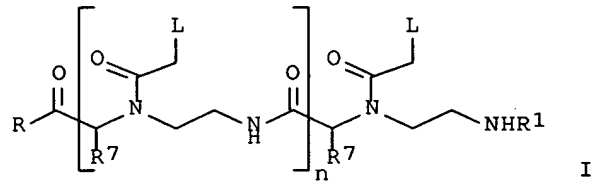

I

AB A novel class of compds., known as peptide nucleic acids (PNAs), e.g. I [each L = independently naturally occurring or non-naturally occurring nucleobase; each R7 = independently H, C1-7 alkylamine, with the proviso that at least one R7 = C1-7 alkylamine; R = OH, NH2, Lys-NH2; R1 = H, Ac, CO2CMe3 (Boc); n = 1-30], bind complementary DNA and RNA strands more strongly than a corresponding DNA strand, and exhibit increased sequence specificity and solubility The peptide nucleic acids comprise ligands selected from a group consisting of naturally-occurring nucleobases and non-naturally-occurring nucleobases attached to a polyamide backbone, and contain alkylamine side chains. Thus, the Tm for PNA H-GTkAGATkCACTk-NH2 (II; aminoethylglycine backbone except where k appears, which is aminoethyl-D-lysine) binding to antiparallel complementary DNA was 55° while that for for PNA H-GTAGATCACT-NH2 (III; with aminoethylglycine backbone) was 52°. The presence of the D-Lys also enhanced sequence specificity: in the presence of a single mismatch in the complementary DNA, the Tm's were 38° and 42° for II and III, resp. A 16-mer PNA containing four lysine side chains was soluble in physiol. useful solns. while the PNA devoid of the lysine side chains was insol. A 12-mer PNA containing two 2,6-diaminopurine nucleobases bearing Lys side chains, prepared by solid-phase methods using Nα-Boc and benzyl side chain protection, blocked in vitro translation of hepatitis C virus protein with EC50 = 29 nM.

IC C12Q001-68

INCL 435006000

CC 34-3 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 1, 6, 26

IT 4113-97-7P 5236-60-2P 6214-59-1P 6943-68-6P 13303-10-1P,
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137618-48-5P 139166-79-3P 139166-80-6P 139166-81-7P 139166-82-8P
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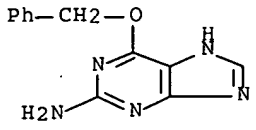
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of peptide nucleic acids having enhanced binding affinity, sequence specificity and solubility)

IT ***19916-73-5P***
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of peptide nucleic acids having enhanced binding affinity, sequence specificity and solubility)

RN 19916-73-5 CAPLUS
CN 9H-Purin-2-amine, 6-(phenylmethoxy)- (CA INDEX NAME)



L18 ANSWER 23 OF 41 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1998:146586 CAPLUS Full-text
DOCUMENT NUMBER: 128:192941
TITLE: Preparation of peptide nucleic acids having enhanced binding affinity, sequence specificity and solubility
INVENTOR(S): Buchardt, Ole; Egholm, Michael; Nielsen, Peter Eigil; Berg, Rolf Henrik
PATENT ASSIGNEE(S): Den.
SOURCE: U.S., 70 pp., Cont.-in-part of U.S. Ser. No. 108,591.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 19
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5719262	A	19980217	US 1996-685484	19960724
US 6395474	B1	20020528	US 1993-108591	19931122
US 5773571	A	19980630	US 1996-595387	19960201
US 5786461	A	19980728	US 1997-847095	19970501
CA 2261566	A1	19980129	CA 1997-2261566	19970724
WO 9803542	A1	19980129	WO 1997-US12811	19970724
W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AN				
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AU 9738081	A	19980210	AU 1997-38081	19970724

AU 717387	B2	20000323			
EP 960121	A1	19991201	EP 1997-935053		19970724
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI					
JP 2000503671	T	20000328	JP 1998-507186		19970724
JP 3306073	B2	20020724			
JP 2002105059	A	20020410	JP 2001-222248		19970724
AT 311402	T	20051215	AT 1997-935053		19970724
US 6710164	B1	20040323	US 1999-230088		19990310
US 2006160731	A1	20060720	US 2003-691012		20031022
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			DK 1991-987	A	19910524
			DK 1992-510	A	19920415
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			US 1997-51002P	P	19970529
			JP 1998-507186	A3	19970724
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OTHER SOURCE(S): MARPAT 128:192941

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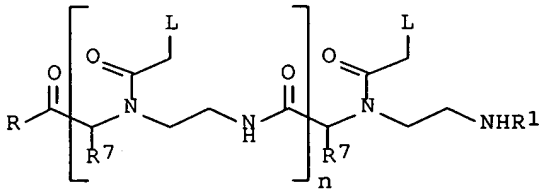

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AB A novel class of compds., known as peptide nucleic acids (PNAs), e.g. I [each L = independently naturally occurring or non-naturally occurring nucleobase; each R7 = independently H, C1-7 alkylamine, with the proviso that at least one R7 = C1-7 alkylamine; R = OH, NH2, Lys-NH2; R1 = H, Ac, CO2CMe3 (Boc); n = 1-30], bind complementary DNA and RNA strands more strongly than a corresponding DNA strand, and exhibit increased sequence specificity and solubility The peptide nucleic acids comprise ligands selected from a group consisting of naturally-occurring nucleobases and non-naturally-occurring nucleobases attached to a polyamide backbone, and contain alkylamine side chains. Thus, a 12-mer PNA containing two 2,6-diaminopurine nucleobases bearing Lys sidechains, prepared by solid-phase methods using Nα-Boc and benzyl side chain protection, blocked in vitro translation of hepatitis C virus protein with EC50 = 29 nM.

IC ICM C12Q001-68
ICS C07H021-00; C07K005-00

INCL 530300000

CC 34-3 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 1, 6, 26

IT 4113-97-7P 5236-60-2P 6214-59-1P 6943-68-6P 13303-10-1P,

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RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of peptide nucleic acids having enhanced binding affinity, sequence specificity and solubility)

IT ***19916-73-5P***
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
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RN 19916-73-5 CAPLUS
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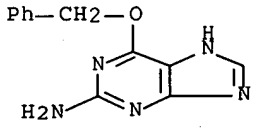

REFERENCE COUNT: 157 THERE ARE 157 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 24 OF 41 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1998:89263 CAPLUS Full-text
DOCUMENT NUMBER: 128:180668
TITLE: Preparation of peptide nucleic acids having enhanced binding affinity, sequence specificity and solubility
INVENTOR(S): Nielsen, Peter E.; Egholm, Michael; Berg, Rolf H.
PATENT ASSIGNEE(S): Buchardt, Dorte, Den.; Isis Pharmaceuticals, Inc.
SOURCE: PCT Int. Appl., 150 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 19
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9803542	A1	19980129	WO 1997-US12811	19970724

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US 5719262	A	19980217	US 1996-685484		19960724
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US 6414112	B1	20020702	US 1996-686114		19960724
AU 9738081	A	19980210	AU 1997-38081		19970724
AU 717387	B2	20000323			
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JP 3306073	B2	20020724			
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US 6107470	A	20000822	US 1999-225146		19990104
US 6710164	B1	20040323	US 1999-230088		19990310
PRIORITY APPLN. INFO.:			US 1996-685484	A	19960724
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			DK 1991-986	A	19910524
			DK 1991-987	A	19910524
			DK 1992-510	A	19920415
			US 1993-108591	A2	19931122
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			US 1998-69705	A1	19980429

OTHER SOURCE(S): MARPAT 128:180668
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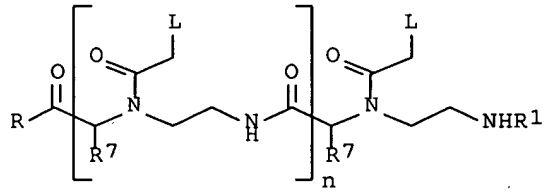

I

AB A novel class of compds., known as peptide nucleic acids (PNAs), e.g. I [each L = independently naturally occurring or non-naturally occurring nucleobase; each R7 = independently H, C1-7 alkylamine, with the proviso that at least one R7 = C1-7 alkylamine; R = OH, NH2, Lys-NH2; R1 = H, Ac, CO2CMe3 (Boc); n = 1-30], bind complementary DNA and RNA strands more strongly than a corresponding DNA strand, and exhibit increased sequence specificity and solubility The peptide nucleic acids comprise ligands selected from a group consisting of naturally-occurring nucleobases and non-naturally-occurring nucleobases attached to a polyamide backbone, and contain C1-C8 alkylamine side chains. Methods of enhancing the solubility, binding affinity and sequence specificity of PNAs are provided. Thus, a 12-mer PNA containing two 2,6-diaminopurine

nucleobases bearing Lys sidechains, prepared by solid-phase methods using Nα-Boc and benzyl side chain protection, blocked in vitro translation of hepatitis C virus protein with EC50 = 29 nM.

IC ICM C07K005-02

CC 34-3 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 1, 6, 26

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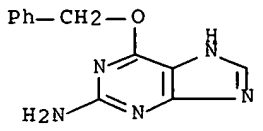
RN 19916-73-5 CAPLUS

CN 9H-Purin-2-amine, 6-(phenylmethoxy)- (CA INDEX NAME)



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 25 OF 41 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1997:807301 CAPLUS Full-text

DOCUMENT NUMBER: 128:61476

TITLE: Facilitation of displacements at the 6-position of purines by the use of 1,4-diazabicyclo[2.2.2]octane as leaving group. [Erratum to document cited in CA126:251122]

AUTHOR(S): Lembicz, Nicola K.; Grant, Sharon; Clegg, William; Griffin, Roger J.; Heath, Sarah L.; Golding, Bernard

T.
CORPORATE SOURCE: Dep. Chem., Univ. Newcastle upon Tyne, Newcastle upon Tyne, NE1 7RU, UK
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1997), (23), 3573
CODEN: JCPRB4; ISSN: 0300-922X
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English

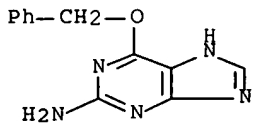
AB The ability of 1,4-diazabicyclo[2.2.2]octane (DABCO) to catalyze reactions of 2-amino-9-benzyl-6-chloro-9H-purine with alkoxides has been demonstrated (J. A. Linn, E. W. McLean and J. L. Kelley, J. Chemical Society, Chemical Commun., 1994, 913). These authors also characterized 1-1-(2-amino-9-benzyl-9H-purin-6-yl)-4-aza-1-azoniabicyclo[2.2.2]octane chloride from reaction of DABCO with 2-amino-9-benzyl-6-chloro-9H-purine in DMF. DABCO has been shown to catalyze reactions or 6-chloropurines with cyanide (M. Hocek and A. Holy, Collect. Czech. Chemical Commun., 1995, 60, 1386).

CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))

IT ***19916-73-5P*** 20535-83-5P 50663-54-2P 161058-83-9P 162320-37-8P 188680-41-3P 188680-42-4P 188680-43-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and substitution reaction of diazabicyclooctane purines (Erratum))

IT ***19916-73-5P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and substitution reaction of diazabicyclooctane purines (Erratum))

RN 19916-73-5 CAPLUS
CN 9H-Purin-2-amine, 6-(phenylmethoxy)- (CA INDEX NAME)



L18 ANSWER 26 OF 41 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1997:687648 CAPLUS Full-text
DOCUMENT NUMBER: 127:342821
TITLE: Substrate Specificity of Human O6-Methylguanine-DNA Methyltransferase for O6-Benzylguanine Derivatives in Oligodeoxynucleotides
AUTHOR(S): Terashima, Isamu; Kawate, Hisaya; Sakumi, Kunihiko; Sekiguchi, Mutsuo; Kohda, Kohfuku
CORPORATE SOURCE: Faculty of Pharmaceutical Sciences, Nagoya City University, Nagoya, 467, Japan
SOURCE: Chemical Research in Toxicology (1997), 10(11), 1234-1239
CODEN: CRTOEC; ISSN: 0893-228X
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB To investigate the substrate specificity of human O6-methylguanine-DNA methyltransferase (MGMT) for O6-benzylguanine (6BG) derivs. incorporated in oligodeoxynucleotides, we prepared 25-mer lengths of sequences containing

various 6BG derivs. and their related compds. and then measured the ability of these derivs. to inactivate MGMT in vitro. Oligodeoxynucleotides containing a 6BG, O6-(2-fluorobenzyl)guanine (2F-6BG), O6-(3-fluorobenzyl)guanine (3F-6BG), O6-(4-fluorobenzyl)guanine (4F-6BG), O6-benzylhypoxanthine (6BH), or O6-methylguanine (6MG) were all good substrates for MGMT, and no obvious differences were observed among them. Oligodeoxynucleotides containing N2-isobutyrated 6BG and 6MG showed only a slightly reduced capacity for inactivating MGMT compared to N2-nonmodified forms of these derivs. No obvious differences were observed in the corresponding double-stranded and single-stranded oligodeoxynucleotides. MGMT substrate specificity for the 6BG derivs. in the oligodeoxynucleotide was found to be quite different from that seen in our previous study. In brief, (i) 6BG, 3F-6BG, and 4F-6BG greatly inhibited human MGMT, whereas 2F-6BG, 6BH, and 6MG displayed much weaker activity; (ii) any modifications at the 2-amino group of the 6BG resulted in severe redns. in the ability to inactivate MGMT. These results obtained by the expts. using oligodeoxynucleotides and free bases suggest that human MGMT has low substrate specificity for 6BGs in oligodeoxynucleotides. Conformational changes in human MGMT which favor binding to oligodeoxynucleotides containing 6BG derivs. and the subsequent transfer of their benzyl groups may account for the difference in substrate specificity between the incorporated 6BG derivs. and their free base form.

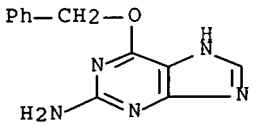
CC 4-6 (Toxicology)

IT ***19916-73-5DP***, O6-Benzylguanine, derivs.
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and substrate specificity of human methylguanine-DNA methyltransferase for benzylguanine derivs. in oligodeoxynucleotides)

IT ***19916-73-5DP***, O6-Benzylguanine, derivs.
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and substrate specificity of human methylguanine-DNA methyltransferase for benzylguanine derivs. in oligodeoxynucleotides)

RN 19916-73-5 CAPLUS

CN 9H-Purin-2-amine, 6-(phenylmethoxy)- (CA INDEX NAME)



REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 27 OF 41 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1997:136347 CAPLUS Full-text

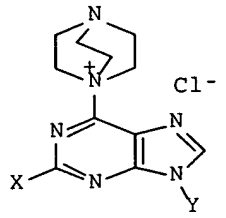
DOCUMENT NUMBER: 126:251122

TITLE: Facilitation of displacements at the 6-position of purines by the use of 1,4-diazabicyclo[2.2.2]octane as leaving group

AUTHOR(S): Lembicz, Nicola K.; Grant, Sharon; Clegg, William; Griffin, Roger J.; Heath, Sarah L.; Golding, Bernard T.

CORPORATE SOURCE: Dep. Chem., Univ. Newcastle upon Tyne, Newcastle upon Tyne, NE1 7RU, UK

SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1997), (3), 185-186
CODEN: JCPRB4; ISSN: 0300-922X
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 126:251122
GI



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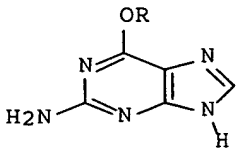


II

AB Reactions of 6-chloropurines with 1,4-diazabicyclo[2.2.2]octane (DABCO) give the corresponding 'DABCO-purines' I (X = NH2, H, Cl, Y = H; X = NH2, Y = β-D-ribofuranosyl), which undergo facile displacement reactions with alkoxides in DMSO to afford 6-oxy-substituted purines II (R = Me, allyl, CH2Ph, cyclohexylmethyl, 2-thienylmethyl, etc.).

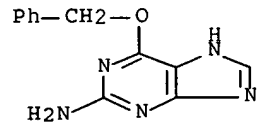
CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))

IT ***19916-73-5P*** 20535-83-5P 50663-54-2P 161058-83-9P 162320-37-8P 188680-41-3P 188680-42-4P 188680-43-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and substitution reaction of diazabicyclooctane purines)

IT ***19916-73-5P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and substitution reaction of diazabicyclooctane purines)

RN 19916-73-5 CAPLUS

CN 9H-Purin-2-amine, 6-(phenylmethoxy)- (CA INDEX NAME)



REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

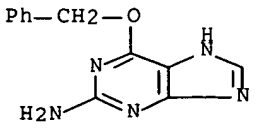
L18 ANSWER 28 OF 41 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1996:411082 CAPLUS Full-text
DOCUMENT NUMBER: 125:143233
TITLE: Process for the preparation of [1R-(1α,2β,3α)]-2-amino-9-[2,3-bis(hydroxymethyl)cyclobutyl]-1,9-dihydro-6H-purin-6-one antiviral agent
INVENTOR(S): Godfrey, Jollie D., Jr.; Mueller, Richard H.; Kissick,

Thomas P.; Singh, Janak
PATENT ASSIGNEE(S): E. R. Squibb and Sons, Inc., USA
SOURCE: U.S., 9 pp., Cont.-in-part of U.S. Ser. No. 961,805, abandoned.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5525726	A	19960611	US 1993-150308	19931112
US 5185463	A	19930209	US 1991-770191	19911002
PRIORITY APPLN. INFO.:			US 1991-770191 A3	19911002
			US 1992-961805 B2	19921016

AB Racemic Feist's acid is treated with (R)-(+)-α-methylbenzylamine to yield (1R-trans)-3-methylene-cyclopropane-1,2-dicarboxylic acid, (R)-α-methylbenzylamine (1:1) salt. This salt can then be converted to (1R-trans)-3-methylene-1,2-cyclopropanedicarboxylic acid, di-Me ester which is an intermediate in the preparation of the antiviral agent [1R-(1α,2β,3α)]-2-amino-9-[2,3-bis(hydroxymethyl)cyclobutyl]-1,9-dihydro-6H-purin-6-one. The improved process also enables the recovery of racemic Feist's acid from the resolution

IC ICM C07B057-00
ICS C07D473-18; A61K031-52
INCL 544276000
CC 33-9 (Carbohydrates)
IT ***19916-73-5P*** 57476-07-0DP, di-protected 127759-89-1P 132294-19-0P 151593-01-0DP, di-protected 179479-06-2DP, di-protected 179479-07-3DP, di-protected 179605-35-7DP, di-protected 179605-36-8DP, di-protected
RL: SPN (Synthetic preparation); PREP (Preparation)
(process for the preparation of amino(bishydroxymethyl)cyclobutyl dihydropurinone antiviral agent)
IT ***19916-73-5P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(process for the preparation of amino(bishydroxymethyl)cyclobutyl dihydropurinone antiviral agent)
RN 19916-73-5 CAPLUS
CN 9H-Purin-2-amine, 6-(phenylmethoxy)- (CA INDEX NAME)



L18 ANSWER 29 OF 41 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1995:228470 CAPLUS Full-text
DOCUMENT NUMBER: 122:127445
TITLE: Probing the active site and mechanism of action of O6-methylguanine-DNA methyltransferase with substrate analogs (O6-substituted guanines)
AUTHOR(S): Arris, Christine E.; Bleasdale, Christine; Calvert, A. Hilary; Curtin, Nicola J.; Dalby, Christine; Golding,

Bernard T.; Griffin, Roger J.; Lunn, J. Martin; Major, Glenn N.; Newell, David R.
CORPORATE SOURCE: Dep. Chem., Univ. Newcastle, Newcastle upon Tyne, NE1 7RU, UK
SOURCE: Anti-Cancer Drug Design (1994), 9(5), 401-8
CODEN: ACDDEA; ISSN: 0266-9536
PUBLISHER: Oxford University Press
DOCUMENT TYPE: Journal
LANGUAGE: English

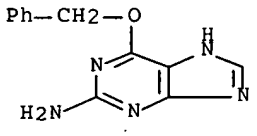
AB A series of O6-(2-oxoalkyl)guanines, their allyl isosteres, and a number of related compds. were synthesized and tested as substrates with O6-methylguanine-DNA methyltransferase. The results support the mechanistic concept outlined previously for the inhibitor O6-benzylguanine and show a dramatic difference between the rates of SN2 reactions for a "pure chemical system" (alkyl halide + iodide in acetone) and a system subject to mol. recognition by a macromol.

CC 7-5 (Enzymes)

IT 73-40-5DP, Guanine, O6-substituted derivs. 6331-91-5P
19916-73-5P 20535-83-5P 50663-54-2P 51866-19-4P
76412-62-9P 161058-73-7P 161058-74-8P 161058-75-9P 161058-76-0P
161058-77-1P 161058-78-2P 161058-79-3P 161058-80-6P 161058-81-7P
161058-82-8P 161058-83-9P 161058-84-0P
RL: BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process)
(methylguanine-DNA methyltransferase specificity and mechanism with O6-substituted guanines)

IT ***19916-73-5P***
RL: BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process)
(methylguanine-DNA methyltransferase specificity and mechanism with O6-substituted guanines)

RN 19916-73-5 CAPLUS
CN 9H-Purin-2-amine, 6-(phenylmethoxy)- (CA INDEX NAME)



L18 ANSWER 30 OF 41 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1995:227238 CAPLUS Full-text
DOCUMENT NUMBER: 122:1073
TITLE: Benzylated guanine, guanosine and deoxyguanosine compounds possessing alkylguanine-DNA alkyltransferase depleting activity
INVENTOR(S): Moschel, Robert C.; Dolan, M. Eileen; Pegg, Anthony E.
PATENT ASSIGNEE(S): United States Dept. of Health and Human Services, USA
SOURCE: U.S., 19 pp. Cont.-in-part of U.S. 5,091,430.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 4
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5352669	A	19941004	US 1990-616913	19901121
US 492468	A0	19900715	US 1990-492468	19900313
US 5091430	A	19920225		
CA 2078129	A1	19910914	CA 1991-2078129	19910313
CA 2078129	C	19990504		
WO 9113898	A1	19910919	WO 1991-US1680	19910313
W: AU, CA, JP				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, NL, SE				
AU 9175821	A	19911010	AU 1991-75821	19910313
AU 646452	B2	19940224		
EP 523100	A1	19930120	EP 1991-906818	19910313
EP 523100	B1	19960828		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
JP 05504972	T	19930729	JP 1991-507224	19910313
JP 2829440	B2	19981125		
AT 141925	T	19960915	AT 1991-906818	19910313
ES 2091322	T3	19961101	ES 1991-906818	19910313
US 5691307	A	19971125	US 1994-255190	19940607
PRIORITY APPLN. INFO.:			US 1990-492468 A2	19900313
			US 1990-616913 A	19901121
			WO 1991-US1680 A	19910313
			US 1991-805634 A2	19911212
			US 1992-875438 B2	19920429

OTHER SOURCE(S): MARPAT 122:1073

AB O6-benzylated guanine, guanosine, and 2'-deoxyguanosine compds. cause a depletion of O6-alkylguanine-DNA alkyltransferase (AGT) activity in mammalian cells. These compds. may be administered to a host to reduce AGT levels in tumor cells of the host in order to increase host responsiveness to antineoplastic alkylating agents, including chloroethylating agents, such as chloroethylnitrosoureas, for chemotherapeutic treatment of a number of neoplasms. For example, the growth rate of human glioma (SF767) xenografts was determined in mice treated with O6-benzylguanine in combination with meCCNU (NSC 95441); the average size of tumors treated with the combination was 2.6-fold smaller than those treated with meCCNU alone.

IC ICM A61K031-70
ICS A61K031-52; C07H017-02; C07D473-18

INCL 514045000

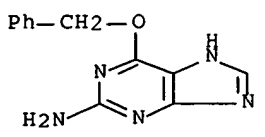
CC 1-6 (Pharmacology)

IT ***19916-73-5P*** 129409-64-9P 129409-65-0P
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(benzylated guanine derivs. and alkylguanine-DNA alkyltransferase depleting activities thereof)

IT ***19916-73-5P***
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(benzylated guanine derivs. and alkylguanine-DNA alkyltransferase depleting activities thereof)

RN 19916-73-5 CAPLUS

CN 9H-Purin-2-amine, 6-(phenylmethoxy)- (CA INDEX NAME)



L18 ANSWER 31 OF 41 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1995:19037 CAPLUS Full-text
DOCUMENT NUMBER: 122:81855
TITLE: Synthesis of N-(3-azido-2-hydroxypropyl), N-(3-phthalimido-2-hydroxypropyl) and N-(3-amino-2-hydroxypropyl) derivatives of heterocyclic bases
AUTHOR(S): Spassova, Maria; Dvorakova, Hana; Holy, Antonin; Budesinsky, Milos; Masojidkova, Milena
CORPORATE SOURCE: Inst. Org. Chem. Biochem., Acad. Sci. Czech Republic, Prague, 166 10, Czech Rep.
SOURCE: Collection of Czechoslovak Chemical Communications (1994), 59(5), 1153-74
CODEN: CCCCAK; ISSN: 0010-0765
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 122:81855
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

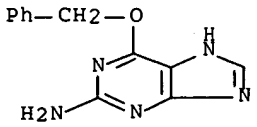
AB Alkylation of heterocyclic bases with azidomethyloxirane (I) under basic catalysis with potassium or cesium carbonate afforded N-(3-azido-2-hydroxypropyl) derivs. BCH2CH(OH)CH2N3 [B = adenin-9-yl, 2,6-diaminopurin-9-yl, 3-deazaadenin-9-yl, 1-deazaadenin-9-yl, 6-chloropurin-9-yl, hypoxanthin-9-yl, guanin-9-yl, 6-(methylmercapto)purin- 9-yl, 6-aminopyrazolo[3,4]pyrimidin-9-yl, 4-methoxy-2-pyrimidon-1-yl, 4-methoxy-5-methyl-2-pyrimidon-1-yl, uracil-1lyl, thymin-1-yl,cytosin-1- yl,6-mercaptopurin-9-yl, 6-mercaptoguanin-9-yl]. Hydrogenation of these compds. over palladium on carbon gave the corresponding 3-amino-2-hydroxypropyl derivs. BCH2CH(OH)CH2NH2. The same compds., BCH2CH(OH)CH2NH2, were prepared by alkylation of heterocyclic bases with phthalimido-methyloxirane (II) in the presence of cesium carbonate and subsequent reaction of the formed N-(3-phthalimido-2-hydroxypropyl) derivs. III with hydrazine. The phthalimido derivs. III are easily hydrolyzed already in weakly alkaline aqueous medium to give 9-[3-(o- carboxybenzoyl-amino)-2-hydroxypropyl] derivs. IV (R1 = Cl, R2 = NH2; R1 = NH2, R2 = H). BCH2CH(OH)CH2R3 (R3 = N3, NH2) were tested for antiviral activity (no data, inactive).

CC 33-9 (Carbohydrates)
Section cross-reference(s): 28

IT ***19916-73-5P***, 2-Amino-6-(benzyloxy)purine 160308-51-0P 160308-52-1P 160308-55-4P 160308-72-5P 160699-98-9P 160699-99-0P
RL: SPN (Synthetic preparation); FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, in preparation of nucleoside analogs)

IT ***19916-73-5P***, 2-Amino-6-(benzyloxy)purine
RL: SPN (Synthetic preparation); FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, in preparation of nucleoside analogs)

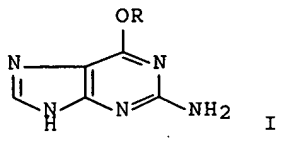
RN 19916-73-5 CAPLUS
CN 9H-Purin-2-amine, 6-(phenylmethoxy)- (CA INDEX NAME)



L18 ANSWER 32 OF 41 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1994:533865 CAPLUS Full-text
DOCUMENT NUMBER: 121:133865
TITLE: Preparation of 2-amino-6-alkoxypurines as intermediates for virucides
INVENTOR(S): Sugimura, Hideo; Chikui, Yukio; Akaha, Hiroshi; Kishigami, Masanori; Tsubaki, Myuki; Sugano, Yoshikazu; Ogawa, Yutaka
PATENT ASSIGNEE(S): Nippon Kayaku Kk, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 4 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 06116266	A	19940426	JP 1992-287151	19921002

PRIORITY APPLN. INFO.: JP 1992-287151 19921002
OTHER SOURCE(S): CASREACT 121:133865; MARPAT 121:133865
GI

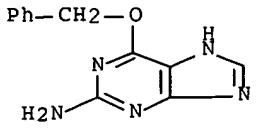


I

AB The title compds. I [R = alkoxyalkyl, alkyl, etc,;] are prepared, e.g., by reaction of 2-amino-6-chloropurine with an alkoxide prepared in situ. A mixture of sodium methoxide 210 g in 7300 mL 2-methoxyethanol was refluxed for 1 h. Approx. 2 Kg 2-methoxyethanol was then evaporated under reduced pressure. The resulting concentrate containing sodium 2-methoxyethanolate was then mixed with 311 g 2-amino-6-chloropurine, and the reaction mixture was refluxed for 3 h to give , after workup, 92 % 2-amino-6-(2-methoxyethoxy)purine.

IC ICM C07D473-18
CC 26-9 (Biomolecules and Their Synthetic Analogs)
IT ***19916-73-5P***, 2-Amino-6-benzyloxypurine 76412-62-9P, 2-Amino-6-butoxypurine 105797-60-2P, 2-Amino-6-(2-methoxyethoxy)purine
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, method for)
IT ***19916-73-5P***, 2-Amino-6-benzyloxypurine
RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of, method for)
RN 19916-73-5 CAPLUS
CN 9H-Purin-2-amine, 6-(phenylmethoxy)- (CA INDEX NAME)



L18 ANSWER 33 OF 41 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1993:581235 CAPLUS Full-text
DOCUMENT NUMBER: 119:181235
TITLE: Peptide nucleic acids
INVENTOR(S): Buchardt, Ole; Egholm, Michael; Nielsen, Peter Eigil; Berg, Rolf Henrik
PATENT ASSIGNEE(S): Den.
SOURCE: PCT Int. Appl., 192 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 19
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9220702	A1	19921126	WO 1992-EP1219	19920522
W: AT, AU, BB, BG, BR, CA, CH, CS, DE, DK, ES, FI, GB, HU, JP, KP, KR, LK, LU, MG, MN, MW, NL, NO, PL, RO, RU, SD, SE, US				
RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FR, GA, GB, GN, GR, IT, LU, MC, ML, MR, NL, SE, SN, TD, TG				
CA 2109320	A1	19921125	CA 1992-2109320	19920522
CA 2109320	C	20030722		
CA 2109805	A1	19921126	CA 1992-2109805	19920522
WO 9220703	A1	19921126	WO 1992-EP1220	19920522
W: AT, AU, BB, BG, BR, CA, CH, CS, DE, DK, ES, FI, GB, HU, JP, KP, KR, LK, LU, MG, MN, MW, NL, NO, PL, RO, RU, SD, SE, US				
RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FR, GA, GB, GN, GR, IT, LU, MC, ML, MR, NL, SE, SN, TD, TG				
AU 9218806	A	19921230	AU 1992-18806	19920522
AU 666480	B2	19960215		
AU 9218843	A	19921230	AU 1992-18843	19920522
EP 586474	A1	19940316	EP 1992-911165	19920522
EP 586474	B1	20010912		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, MC, NL, SE				
EP 586618	A1	19940316	EP 1992-923579	19920522
EP 586618	B1	19970716		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
JP 06506945	T	19940804	JP 1992-510434	19920522
JP 2758988	B2	19980528		
JP 06509063	T	19941013	JP 1992-510139	19920522
BR 9206049	A	19941227	BR 1992-6049	19920522
HU 66597	A2	19941228	HU 1993-3023	19920522
HU 221003	B1	20020729		
AT 155483	T	19970815	AT 1992-923579	19920522
ES 2107552	T3	19971201	ES 1992-923579	19920522

EP 1074559	A1	20010207	EP 2000-203148	19920522
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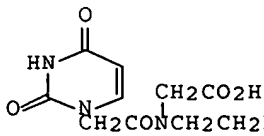
AT 205504	T	20010915	AT 1992-911165	19920522
EP 1162206	A2	20011212	EP 2001-203303	19920522
EP 1162206	A3	20040414		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC				
ES 2164052	T3	20020216	ES 1992-911165	19920522
JP 2003235590	A	20030826	JP 2003-15384	19920522
EP 1411063	A1	20040421	EP 2003-77836	19920522
EP 1411063	B1	20060719		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC				
US 6228982	B1	20010508	US 1993-88661	19930702
NO 9304122	A	19940111	NO 1993-4122	19931115
NO 312516	B1	20020521		
KR 133131	B1	19980414	KR 1993-703558	19931120
US 6395474	B1	20020528	US 1993-108591	19931122
NO 9304235	A	19940120	NO 1993-4235	19931123
NO 313201	B1	20020826		
US 6357163	B1	20020319	US 1994-150156	19940504
US 6451968	B1	20020917	US 1994-275951	19940715
US 5977296	A	19991102	US 1994-366231	19941228
US 6710163	B1	20040323	US 1995-468719	19950606
US 5986053	A	19961116	US 1995-471907	19950607
US 6441130	B1	20020827	US 1998-765798	19980628
US 6770738	B1	20040803	US 1999-442054	19991116
US 6610650	B1	20030826	US 2000-610264	20000706
US 2002160383	A1	20021031	US 2001-983210	20011023
US 2003105286	A1	20030605	US 2002-188404	20020701
US 2003232355	A1	20031218	US 2003-348246	20030121
US 2004059087	A1	20040325	US 2003-657600	20030908
US 2006160731	A1	20060720	US 2003-691012	20031022
US 2005009041	A1	20050113	US 2004-755118	20040109
US 2005048552	A1	20050303	US 2004-909914	20040802
US 2006046255	A1	20060302	US 2005-29005	20050105

PRIORITY APPLN. INFO.:

DK 1991-986	A	19910524
DK 1991-987	A	19910524
DK 1992-510	A	19920415
EP 1992-911165	A3	19920522
EP 2000-203148	A3	19920522
JP 1992-510139	A3	19920522
US 1992-108591	B2	19920522
WO 1992-EP1219	A	19920522
WO 1992-EP1220	A	19920522
US 1993-54363	A2	19930426
US 1993-88658	A2	19930702
US 1993-88661	A2	19930702
US 1993-108591	A2	19931122
US 1994-150156	A1	19940504
US 1994-275951	A2	19940715
US 1995-462977	A1	19950605
US 1995-468719	A3	19950606
US 1995-471907	A3	19950607
WO 1995-US9084	W	19950713
US 1998-765798	A3	19980628
US 1999-442054	A1	19991116
US 2000-610624	A3	20000705
US 2001-983210	B1	20011023
US 2002-154890	A3	20020523

OTHER SOURCE(S): MARPAT 119:181235

GI



I

AB Peptides containing nucleic acid bases were prepared These peptides formed stable hybrids with oligonucleotides. Thus, H2NCH2CH2NHCH2CO2H was tert-butoxycarbonylated and treated with N1-carboxymethylthymine pentafluorophenyl ester to give the thymine derivative Boc-Taeg-OH (I). I was used in the solid-phase synthesis of H-[Taeg]10-Lys-NH2 which formed a hybrid with (dA)10 which had a melting temperature of 73°.

IC ICM C07K005-00
ICS C07K007-00; C12Q001-68; C08L077-00

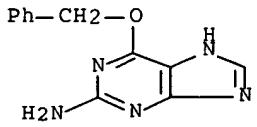
CC 34-3 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 33

IT ***19916-73-5P*** 149411-91-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with bromoacetate)

IT ***19916-73-5P***
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with bromoacetate)

RN 19916-73-5 CAPLUS

CN 9H-Purin-2-amine, 6-(phenylmethoxy)- (CA INDEX NAME)



L18 ANSWER 34 OF 41 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1992:59907 CAPLUS Full-text

DOCUMENT NUMBER: 116:59907

TITLE: O6-benzylated guanine, guanosine and 2-deoxyguanosine compounds possessing O6-alkylguanine-DNA alkyltransferase (AGT) depleting activity

INVENTOR(S): Moschel, Robert Carl; Dolan, Mary Eileen; Pegg, Anthony E.

PATENT ASSIGNEE(S): United States Dept. of Commerce, USA

SOURCE: PCT Int. Appl., 47 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 4

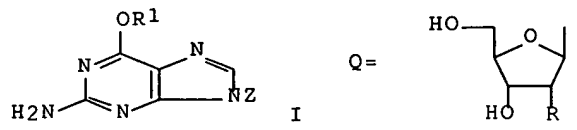
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9113898	A1	19910919	WO 1991-US1680	19910313
W: AU, CA, JP				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, NL, SE				
US 492468	A0	19900715	US 1990-492468	19900313
US 5091430	A	19920225		
US 5352669	A	19941004	US 1990-616913	19901121
AU 9175821	A	19911010	AU 1991-75821	19910313
AU 646452	B2	19940224		
EP 523100	A1	19930120	EP 1991-906818	19910313
EP 523100	B1	19960828		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
JP 05504972	T	19930729	JP 1991-507224	19910313
JP 2829440	B2	19981125		

PRIORITY APPLN. INFO.:	US 1990-492468	A	19900313
	US 1990-616913	A	19901121
	WO 1991-US1680	A	19910313

OTHER SOURCE(S): MARPAT 116:59907

GI



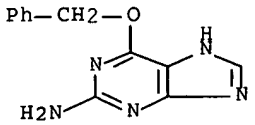
AB The title compds. [I; Z = H, Q; R = H, OH; R1 = benzyl substituted at the o-, m-, or p-position with halo, NO2, (un)substituted Ph, C1-4 alkyl, C1-4 alkoxy, C≤4 alkenyl or alkynyl, (mono- or dialkyl)amino, CF3, OH, CH2OH, or S(O)nR2; n = 0, 1, 2; R2 = H, C1-4 alkyl, (un)substituted Ph] are prepared I are administered to a host so as to reduce AGT levels in tumor cells of the host in order to increase host responsiveness to antineoplastic alkylating agents, e.g. chloroethylnitrosoureas, for chemotherapeutic treatment of neoplasms. Thus, O6-benzylguanine (II) was prepared by treating 0.018 mol 2-amino-6-chloropurine with 2.2 equivalent PhCH2ONa in 30 g PhCH2OH at 130° for 24 h. II efficiently depleted the alkyltransferase activity in vitro against human AGT and in HT29 cells and in vivo in CD-1 mice and hamsters. Cytotoxicity of clomesone or 1-(2-chloroethyl)-3-cyclohexyl-1-nitrosourea (lomustine, CCNU) against HT29 cells was markedly increased in the presence of 10 μM II, while II alone showed no cytotoxicity at ≤100 μM. Furthermore, the growth rate of human glioma SF767 tumor xenografts in nude mice was 1.6 fold greater in volume in control animals than those in MeCCNU (NSC 95441) (7.5 mg/kg)-treated animals and 3.7 fold larger in animals treated with both I (60 mg/kg) and MeCCNU (7.5 mg/kg) on day 21. Also prepared and tested were O6-p-chlorobenzyl-, p-methylbenzyl-, or p-fluorobenzylguanine and O6-benzyl-2'-deoxyguanosine. They were more active than O6-methylguanine for alkyltransferase inactivation.

IC ICM C07H017-00
ICS C07D473-00; A61K031-52; A61K031-70

CC 33-9 (Carbohydrates)
Section cross-reference(s): 1, 7

IT ***19916-73-5P***, O6-Benzylguanine 67733-78-2P 129409-64-9P

129732-90-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and alkylguanine-DNA alkyltransferase of animal tissue and neoplasm depletion by, antitumor sensitivity in relation to)
IT *19916-73-5P*, O6-Benzylguanine
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and alkylguanine-DNA alkyltransferase of animal tissue and neoplasm depletion by, antitumor sensitivity in relation to)
RN 19916-73-5 CAPLUS
CN 9H-Purin-2-amine, 6-(phenylmethoxy)- (CA INDEX NAME)

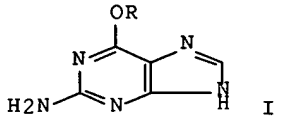


L18 ANSWER 35 OF 41 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1991:75204 CAPLUS Full-text
DOCUMENT NUMBER: 114:75204
TITLE: O6-substituted guanine compounds and methods for depleting O6-alkylguanine DNA transferase levels for neoplasm inhibitor enhancement
INVENTOR(S): Moschel, Robert C.; Dolan, E. E.; Pegg, Anthony E.
PATENT ASSIGNEE(S): National Institutes of Health, USA
SOURCE: U. S. Pat. Appl., 29 pp. Avail. NTIS Order No. PAT-APPL-7-492 468.
CODEN: XAXXAV
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 4
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 492468	A0	19900715	US 1990-492468	19900313
US 5091430	A	19920225		
US 5352669	A	19941004	US 1990-616913	19901121
CA 2078129	A1	19910914	CA 1991-2078129	19910313
CA 2078129	C	19990504		
WO 9113898	A1	19910919	WO 1991-US1680	19910313
W: AU, CA, JP				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, NL, SE				
AU 9175821	A	19911010	AU 1991-75821	19910313
AU 646452	B2	19940224		
EP 523100	A1	19930120	EP 1991-906818	19910313
EP 523100	B1	19960828		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
JP 05504972	T	19930729	JP 1991-507224	19910313
JP 2829440	B2	19981125		
AT 141925	T	19960915	AT 1991-906818	19910313
ES 2091322	T3	19961101	ES 1991-906818	19910313
US 5358952	A	19941025	US 1991-805634	19911212
US 5691307	A	19971125	US 1994-255190	19940607
PRIORITY APPLN. INFO.:			US 1990-492468 A2	19900313
			US 1990-616913 A	19901121

WO 1991-US1680	A	19910313
US 1991-805634	A2	19911212
US 1992-875438	B2	19920429

OTHER SOURCE(S): MARPAT 114:75204
GI



I

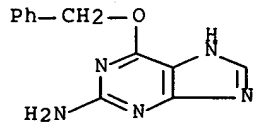
AB The title compds. I [R = (substituted)benzene] are provided for effectively reducing O6-alkylguanine DNA alkyltransferase (II) levels in tumor cells. Also provided are methods for increasing host responsiveness to anti-neoplastic chloroethylating agents or other alkylating agents by administration of compns. containing I. Thus, in vitro exposure of II to 0.25 μM O6-benzylguanine (III) for 30 min led to a loss of >50% of II activity, and exposure to ≥2.5 μM III completely inactivated II; the loss of activity was irreversible. Exposure of human colon carcinoma cell line HT29 to III led to the efficient depletion of II activity. The reduction of II in HT29 cells by III led to a marked increase in the cytotoxicity of either 1-(2-chloroethyl)-3-cyclohexyl-1-nitrosourea or clomesone; exposure to III alone showed no tonic effects at doses <100 μM for 24 h.

CC 1-6 (Pharmacology)
Section cross-reference(s): 7

IT ***19916-73-5P*** 129409-64-9P 129409-65-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as alkylguanine DNA alkyltransferase inhibitor for neoplasm
inhibitor enhancement)

IT ***19916-73-5P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as alkylguanine DNA alkyltransferase inhibitor for neoplasm
inhibitor enhancement)

RN 19916-73-5 CAPLUS
CN 9H-Purin-2-amine, 6-(phenylmethoxy)- (CA INDEX NAME)



L18 ANSWER 36 OF 41 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1986:515383 CAPLUS Full-text
DOCUMENT NUMBER: 105:115383
TITLE: Regioselective synthesis of 9-substituted purine

acyclonucleoside derivatives

INVENTOR(S): Maccoss, Malcolm; Tolman, Richard L.; Wagner, Arthur F.; Hannah, John

PATENT ASSIGNEE(S): Merck and Co., Inc. , USA

SOURCE: Eur. Pat. Appl., 36 pp.
CODEN: EPXXDW

DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 184473	A1	19860611	EP 1985-402031	19851021
R: CH, DE, FR, GB, IT, LI, NL				
JP 61109796	A	19860528	JP 1985-239273	19851025
US 4801710	A	19890131	US 1988-153539	19880202
PRIORITY APPLN. INFO.:			US 1984-665409 A	19841026

OTHER SOURCE(S): CASREACT 105:115383; MARPAT 105:115383

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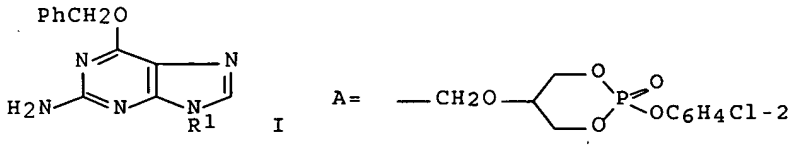


AB Guanine-related acyclonucleosides were prepared Purine derivative I (R1 = H) was treated with NaH and a 5-(chloromethoxy)-1,3,2-dioxaphosphorinane 2-oxide derivative to give I (R1 = A).

IC ICM C07D473-18
ICS C07F009-65; C07D473-40

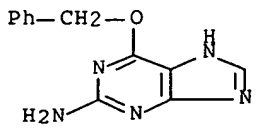
CC 33-9 (Carbohydrates)

IT ***19916-73-5P*** 34798-95-3P 104121-17-7P 104121-18-8P 104121-19-9P 104121-25-7P 104121-30-4P 104121-31-5P 104140-60-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of)

IT ***19916-73-5P***
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of)

RN 19916-73-5 CAPLUS

CN 9H-Purin-2-amine, 6-(phenylmethoxy)- (CA INDEX NAME)



L18 ANSWER 37 OF 41 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1985:523842 CAPLUS Full-text
DOCUMENT NUMBER: 103:123842
TITLE: Synthesis of the chiral acyclonucleoside antiherpetic agent (S)-9-(2,3-dihydroxy-1-propoxymethyl)guanine
AUTHOR(S): MacCoss, Malcolm; Chen, Anna; Tolman, Richard L.
CORPORATE SOURCE: Merck Sharp and Dohme Res. Lab., Rahway, NJ, 07065, USA
SOURCE: Tetrahedron Letters (1985), 26(15), 1815-18
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 103:123842
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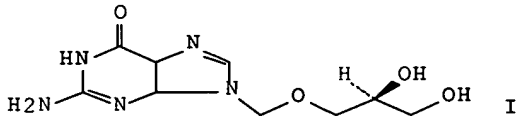


I

AB The title compound (I) was prepared from Me 2,3,4-tri-O-benzyl-α-D-glucopyranoside. The sequence utilizes the absolute configuration defined by carbons 4, 5 and 6 of the D-glucose ring and provides a ready synthesis of the single enantiomer without recourse to many chromatog. sepns.

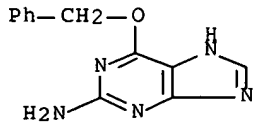
CC 33-9 (Carbohydrates)

IT ***19916-73-5P***
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with chloromethylated Me glucopyranoside derivative)

IT ***19916-73-5P***
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with chloromethylated Me glucopyranoside derivative)

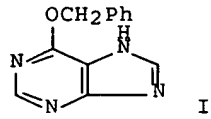
RN 19916-73-5 CAPLUS

CN 9H-Purin-2-amine, 6-(phenylmethoxy)- (CA INDEX NAME)



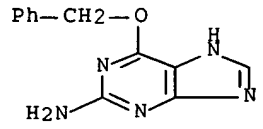
L18 ANSWER 38 OF 41 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1977:115995 CAPLUS Full-text
DOCUMENT NUMBER: 86:115995

TITLE: Cytokinin activity of O6-substituted guanine and hypoxanthine derivatives
AUTHOR(S): Hashizume, Takeshi; Sakai, Sadakatsu; Sugiyama, Tamizi; Matsubara, Satoshi
CORPORATE SOURCE: Lab. Bioorg. Chem., Tokyo Univ. Agric. Technol., Tokyo, Japan
SOURCE: Phytochemistry (Elsevier) (1976), 15(12), 1813-15
CODEN: PYTCAS; ISSN: 0031-9422
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



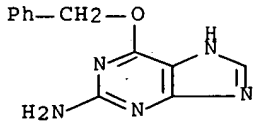
I

AB Of 8 O6-substituted guanine and hypoxanthine derivs. prepared and tested for their cytokinin activity relative to kinetin on tobacco callus, lettuce seeds, and radish cotyledons, O6-benzylhypoxanthine (I) [57500-07-9] was the most active. Guanine derivs. were generally less active than the corresponding hypoxanthine derivs.
CC 5-3 (Agrochemicals)
Section cross-reference(s): 28
IT 5454-70-6P ***19916-73-5P*** 57500-07-9P 62134-29-6P 62134-30-9P 62134-31-0P 62134-32-1P 62134-33-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and cytokinin activity of)
IT ***19916-73-5P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and cytokinin activity of)
RN 19916-73-5 CAPLUS
CN 9H-Purin-2-amine, 6-(phenylmethoxy)- (CA INDEX NAME)



L18 ANSWER 39 OF 41 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1974:14899 CAPLUS Full-text
DOCUMENT NUMBER: 80:14899
TITLE: Allylic rearrangement from O6 to C-8 in the guanine series
AUTHOR(S): Frihart, Charles R.; Leonard, Nelson J.
CORPORATE SOURCE: Sch. Chem. Sci., Univ. Illinois, Urbana, IL, USA
SOURCE: Journal of the American Chemical Society (1973),

95(21), 7174-5
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB Reaction of 2-amino-6-chloropurine (I) with allylic alkoxides gave 8-substituted guanines (II, R = allylic group) instead of O6-substituted guanines. The O6 ether was shown to be an intermediate, and the overall result can be viewed as a combined Claisen-Cope rearrangement via C-5 involving two [3,3] sigmatropic shifts. The O6 to C-8 rearrangement occurs without overall allylic inversion, is partially controlled by the degree of Me substitution on the allylic group and by the temperature, and proceeds with greatest facility through anionic species. The O6-methyl, -ethyl, and -benzyl derivs. of guanine do not undergo this rearrangement under equivalent conditions. In the reaction of I with Na benzyloxide (II) to form the O6-benzylguanine, when excess II and a trace of BzH were used, the product was N2- rather than O6-benzylguanine.
CC 28-19 (Heterocyclic Compounds (More Than One Hetero Atom))
IT ***19916-73-5P***
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and rearrangement of)
IT ***19916-73-5P***
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and rearrangement of)
RN 19916-73-5 CAPLUS
CN 9H-Purin-2-amine, 6-(phenylmethoxy)- (CA INDEX NAME)



L18 ANSWER 40 OF 41 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1969:439386 CAPLUS Full-text
DOCUMENT NUMBER: 71:39386
TITLE: Purine nucleosides. XXIV. A new method for the synthesis of guanine nucleosides. Preparation of 21-deoxy-α- and -β-guanosines and the corresponding N2-methyl derivatives
AUTHOR(S): Robins, Morris J.; Robins, Roland K.
CORPORATE SOURCE: Univ. of Utah, Salt Lake City, UT, USA
SOURCE: Journal of Organic Chemistry (1969), 34(7), 2160-3
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Diazotization of 2-amino-6-(benzyloxy)purine in HBF4 produced 2-fluoro-6-(benzyloxy)purine (I). Acid-catalyzed fusion of I with 1,3,5-tri-O-acetyl-2-deoxy-D-erythro-pentofuranose gave the anomeric 2-fluoro-6-(benzyloxy)-9-(3,5-di-O-acetyl-2-deoxy-D-erythro- pentofuranosyl)purines. Treatment of this mixture with alc. NH3 (or MeNH2) provided the 2-amino-(or 2-(methylamino))-6-(benzyloxy)-9-(2-deoxy-α-

and -β-D-erythro - pentofuranosyl)purines which were resolved into pure anomers by chromatog. on Dowex 1-X2. Pd/C-catalyzed hydrogenation of these benzyloxy derivs. gave the desired guanine 2'-deoxynucleosides, which obey Hudson's isorotation rules. The N.M.R. spectra of these 2'-deoxy-D-erythro-pentofuranosides had a peak corresponding to an A2X system which appeared as a "triplet" with JH1" = 7 Hz. for the β-anomer and a "quartet" with JH1' .simeq. 3.5 and 7.5 Hz. for the α-anomer. A facile synthesis of 2-amino-6-(benzyloxy)purine from 2,4,5-triamino-6-(benzyloxy)pyrimidine is described. Alternative binding mechanisms of actinomycin D to DNA are considered with respect to N2-methyl-2'-deoxyguanosine.

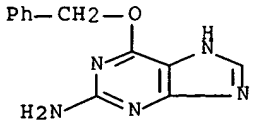
CC 34 (Synthesis of Amino Acids, Peptides, and Proteins)

IT 73-40-5DP, Guanine, nucleosides 961-07-9P 19916-72-4P
19916-73-5P 19916-74-6P 19916-75-7P 19916-77-9P
19916-78-0P 19916-79-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

IT ***19916-73-5P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 19916-73-5 CAPLUS

CN 9H-Purin-2-amine, 6-(phenylmethoxy)- (CA INDEX NAME)



L18 ANSWER 41 OF 41 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1963:448352 CAPLUS Full-text

DOCUMENT NUMBER: 59:48352

ORIGINAL REFERENCE NO.: 59:8736c-e

TITLE: Synthesis and antitumor activity of 9-(tetrahydro-2-furyl)-purine analogs of biologically important deoxynucleosides

AUTHOR(S): Bowles, William A.; Schneider, F. Howard; Lewis, Leland R.; Robins, Roland K.

CORPORATE SOURCE: Arizona State Univ., Tempe

SOURCE: Journal of Medicinal Chemistry (1963), 6(5), 471-80
CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

OTHER SOURCE(S): CASREACT 59:48352

GI For diagram(s), see printed CA Issue.

AB The syntheses of the 9-(tetrahydro-2-furyl) derivs. of hypoxanthine, guanine, and 2-amino-6-purinethiol (6-thioguanine) have been accomplished. The reaction of 2,3-dihydro-2-methylfuran with 6-chloropurine has been studied. Several of the 9-(tetrahydro-2-furyl) purines (I) exhibit significant antitumor activity against a variety of exptl. mouse tumors. The significance of these results is discussed in terms of therapeutic index, transport, and structural relationship to various purine-2'-deoxynucleosides and other biol. active purine derivs.

CC 38 (Heterocyclic Compounds (More Than One Hetero Atom))

IT 118-92-3P, Anthranilic acid, esters with Et lactate 118-92-3P, Anthranilic acid, esters with Et lactate, picrate 735-28-4P,

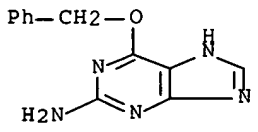
o-Benzotoluidide, 2-amino-α,α,α-trifluoro- 4943-85-5P, o-Benzotoluidide, 2-amino- 7602-01-9P, Purine, 2-acetamido-6-chloro- 19562-43-7P, p-Benzophenetidide, 2-amino- ***19916-73-5P***, Purine, 2-amino-6-(benzyloxy)- 30924-37-9P, Anthranilic acid, p-chlorophenyl ester 32212-38-7P, p-Benzotoluidide, 2-amino- 33708-96-2P, Anthranilic acid, benzyl ester, hydrochloride 40297-58-3P, 9H-Purine-6-thiol, 9-(tetrahydro-5-methyl-2-furyl)- 52745-20-7P, Pyrrolidine, 1-anthraniloyl- 57500-07-9P, Purine, 6-(benzyloxy)- 70083-21-5P, o-Benzanisidide, 2-amino- 82185-41-9P, Anthranilic acid, benzyl ester 82422-32-0P, Anthranilic acid, thio-, S-benzyl ester 84362-82-3P, Anthranilic acid, hexadecyl ester 84362-82-3P, 1-Hexadecanol, anthranilate 85819-70-1P, Guanine, 9-(tetrahydro-2-furyl)- 90348-54-2P, 9H-Purine, 2,6-dichloro-9-(tetrahydro-2-furyl)- 90408-20-1P, Phenol, p-bromo-, anthranilate 90408-20-1P, Anthranilic acid, p-bromophenyl ester 90537-04-5P, Anthranilic acid, 2,2,2-tribromoethyl ester, hydrochloride 90537-05-6P, Anthranilic acid, 2,2,2-tribromoethyl ester 90537-05-6P, Ethanol, 2,2,2-tribromo-, anthranilate 90559-89-0P, 9H-Purine-6-thiol, 2-amino-9-(tetrahydro-2-furyl)- 90794-98-2P, 9H-Purine, 6-chloro-9-(tetrahydro-5-methyl-2-furyl)- 90875-00-6P, Anthranilic acid, thio-, S-isopropyl ester 90875-01-7P, Anthranilic acid, thio-, S-propyl ester 90923-98-1P, Anthranilic acid, 2-propynyl ester, hydrochloride 90923-99-2P, Anthranilic acid, 2-propynyl ester 90923-99-2P, 2-Propyn-1-ol, anthranilate 91090-24-3P, 9H-Purine, 2-acetamido-6-chloro-9-(tetrahydro-2-furyl)- 91247-62-0P, Anthranilic acid, 2-ethoxyethyl ester 91247-62-0P, Ethanol, 2-ethoxy-, anthranilate 91337-65-4P, Piperazine, 1-anthraniloyl- 91563-50-7P, Anthranilic acid, thio-, S-pentyl ester, hydrochloride 91563-51-8P, Anthranilic acid, thio-, S-pentyl ester 91692-65-8P, Anthranilic acid, 2,4,6-tribromophenyl ester, hydrochloride 91692-66-9P, Phenol, 2,4,6-tribromo-, anthranilate 91692-66-9P, Anthranilic acid, 2,4,6-tribromophenyl ester 91956-92-2P, Anthranilic acid, 3-hexynyl ester, hydrochloride 91956-93-3P, Anthranilic acid, 3-hexynyl ester 91956-93-3P, 3-Hexyn-1-ol, anthranilate 91973-54-5P, 3-Pyridinol, anthranilate 91973-54-5P, Anthranilic acid, 3-pyridyl ester 92025-68-8P, Purine, 2-amino-6-(benzylthio)-7-methyl- 92025-71-3P, 9H-Purine, 2-amino-6-(benzylthio)-9-methyl- 92040-41-0P, Anthranilic acid, 3-hexenyl ester, hydrochloride 92040-42-1P, 3-Hexen-1-ol, anthranilate 92040-42-1P, Anthranilic acid, 3-hexenyl ester 92044-43-4P, Anthranilic acid, o-chlorophenyl ester, hydrochloride 92044-44-5P, Anthranilic acid, o-chlorophenyl ester 92044-45-6P, Anthranilic acid, p-chlorophenyl ester, hydrochloride 92059-96-6P, Anthranilic acid, p-bromophenyl ester, hydrochloride 92193-67-4P, Purine, 2-acetamido-6-(benzylthio)- 92193-74-3P, Purine, 2-acetamido-6-(benzyloxy)- 92199-43-4P, Anthranilic acid, o-tolyl ester, hydrochloride 92199-44-5P, Anthranilic acid, o-tolyl ester 92322-30-0P, Anthranilic acid, thio-, S-heptyl ester, hydrochloride 92322-31-1P, Anthranilic acid, thio-, S-heptyl ester 92658-75-8P, Hypoxanthine, 9-(tetrahydro-2-furyl)- 92851-05-3P, Anthranilic acid, o-ethoxyphenyl ester 92851-05-3P, Phenol, o-ethoxy-, anthranilate 93009-81-5P, 9H-Purine, 2-acetamido-9-acetyl-6-(benzylthio)- 93282-13-4P, Adenine, 2-chloro-9-(tetrahydro-2-furyl)- 93312-54-0P, 9H-Purine, 2-amino-6-(benzylthio)-9-(tetrahydro-2-furyl)- 93324-94-8P, 2-Naphthalenethiol, anthranilate 93324-94-8P, Anthranilic acid, thio-, S-2-naphthyl ester 93533-27-8P, Anthranilic acid, m-nitrobenzyl ester 93780-27-9P, Adenine, 9-(tetrahydro-5-methyl-2-furyl)- 93787-25-8P, Adenine, 2-methoxy-9-(tetrahydro-2-furyl)- 93985-57-0P, Anthranilic acid, m-tolyl ester 93988-27-3P, Benzanilide, 2-amino-2',4'-dimethoxy- 94502-90-6P, Anthranilic acid, thio-, S-butyl ester, hydrochloride 94502-91-7P, Anthranilic acid, thio-, S-butyl ester 94571-46-7P, 9H-Purine, 6-(benzyloxy)-9-(tetrahydro-2-furyl)- 94623-44-6P,

Anthranilic acid, α-phenyl-p-tolyl ester 94623-44-6P, p-Cresol, α-phenyl-, anthranilate 94623-69-5P, Phenol, p-(benzyloxy)-, anthranilate 94623-69-5P, Anthranilic acid, p-(benzyloxy)phenyl ester 94960-36-8P, 9H-Purine, 2-acetamido-6-(benzylthio)-9-(tetrahydro-2-furyl)- 94969-83-2P, 1-Tetradecanol, anthranilate 94969-83-2P, Anthranilic acid, tetradecyl ester 94980-49-1P, Adenine, 2-chloro-N-methyl-9-(tetrahydro-2-furyl)- 95289-40-0P, Anthranilic acid, p-(1,1,3,3-tetramethylbutyl)phenyl ester, hydrochloride 95289-41-1P, Anthranilic acid, p-(1,1,3,3-tetramethylbutyl)phenyl ester 95289-41-1P, Phenol, p-(1,1,3,3-tetramethylbutyl)-, anthranilate 95367-89-8P, Anthranilic acid, dodecyl ester 95493-90-6P, Guanine, N-acetyl-9-(tetrahydro-2-furyl)- 95515-96-1P, o-Benzotoluidide, 2-amino-, hydrochloride 96279-28-6P, Ammonium, trimethyl[9-(tetrahydro-5-methyl-2-furyl)-9H-purin-6-yl], chloride 96651-20-6P, Lactic acid, ethyl ester, anthranilate 96875-10-4P, Anthranilic acid, m-nitrobenzyl ester, hydrochloride 97196-87-7P, Anthranilic acid, thio-, S-p-chlorophenyl ester, hydrochloride 97196-88-8P, Anthranilic acid, thio-, S-p-chlorophenyl ester 98090-59-6P, Anthranilic acid, carvacryl ester 98544-17-3P, Anthranilic acid, m-pentadecylphenyl ester, hydrochloride 98544-18-4P, Phenol, m-pentadecyl-, anthranilate 98544-18-4P, Anthranilic acid, m-pentadecylphenyl ester 106041-66-1P, Cholesterol, anthranilate 875830-51-6P, Anthranilic acid, p-tert-pentylphenyl ester 875830-51-6P, Phenol, p-tert-pentyl-, anthranilate 879645-92-8P, Piperazine, 1-anthraniloyl-, picrate 879652-37-6P, p-Benzophenetidide, 2-amino-, picrate 879653-24-4P, p-Benzotoluidide, 2-amino-, picrate 879653-39-1P, o-Benzanisidide, 2-amino-, picrate 879655-48-8P, Anthranilic acid, tetradecyl ester, picrate 879655-71-7P, Anthranilic acid, α-phenyl-p-tolyl ester, picrate 879655-77-3P, Anthranilic acid, tert-pentyl ester, picrate 879655-84-2P, Anthranilic acid, 2-ethoxyethyl ester, compound with 1,3,5-trinitrobenzene 879655-90-0P, Anthranilic acid, carvacryl ester, picrate 879655-98-8P, Anthranilic acid, p-(benzyloxy)phenyl ester, picrate 879656-06-1P, Anthranilic acid, thio-, S-propyl ester, compound with 1,3,5-trinitrobenzene 879656-14-1P, Anthranilic acid, thio-, S-2-naphthyl ester, picrate
RL: PREP (Preparation)
(preparation of)

IT ***19916-73-5P***, Purine, 2-amino-6-(benzyloxy)-
RL: PREP (Preparation)
(preparation of)

RN 19916-73-5 CAPLUS

CN 9H-Purin-2-amine, 6-(phenylmethoxy)- (CA INDEX NAME)



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L2           1 SEA SSS SAM L1
               D SCA
L3          16 SEA SSS FUL L1
               SAVE TEMP L3 BER451STR1L/A
               D SCA
               E 9H-PURIN-2-AMINE, 6-(PHENYLMETHOXY)-/CN
L4           1 SEA ABB=ON  PLU=ON  "9H-PURIN-2-AMINE, 6-(PHENYLMETHOXY)-"/CN
L5          15 SEA ABB=ON  PLU=ON  L3 NOT L4

     FILE 'CAPLUS' ENTERED AT 11:04:28 ON 09 MAR 2007
L6           9 SEA ABB=ON  PLU=ON  L5
L7         451 SEA ABB=ON  PLU=ON  L4

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               SEL RN L4
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L9           0 SEA ABB=ON  PLU=ON  L8 NOT L5

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L11          6 SEA ABB=ON  PLU=ON  L10 AND L6
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L*** DEL     9 S L AND L12
L13          2 SEA ABB=ON  PLU=ON  L6 AND L12

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L14          9 SEA ABB=ON  PLU=ON  L11 OR L6

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L15            ANALYZE PLU=ON  L5 1- LC :       5 TERMS
               D
L16         14 SEA ABB=ON  PLU=ON  L5 AND CAPLUS/LC
L17          1 SEA ABB=ON  PLU=ON  L5 NOT L16
               D SCA
               D LC L17
               D IDE L17

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L18         41 SEA ABB=ON  PLU=ON  L10 NOT L14
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FILE HOME

FILE REGISTRY
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FILE LAST UPDATED: 8 Mar 2007 (20070308/ED)

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